

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102624\
 Data File : BF140064.D
 Acq On : 26 Oct 2024 17:16
 Operator : RC/JU
 Sample : P4471-02
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 B-180-SB02

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Filtering: 5

Sampling : 1

Min Area: 3 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF140064.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.216	12	21	28	rVB	1379832	2208512	51.40%	5.450%
2	5.116	506	514	522	rVB	132492	203577	4.74%	0.502%
3	5.510	574	581	586	rBV	1946641	2748899	63.98%	6.783%
4	6.069	671	676	681	rVB	37611	47318	1.10%	0.117%
5	6.175	688	694	700	rVB	3171045	4296457	100.00%	10.602%
6	6.340	715	722	727	rVB2	127377	260291	6.06%	0.642%
7	6.440	734	739	744	rBV2	46076	69578	1.62%	0.172%
8	6.504	744	750	756	rBV	1889536	2746184	63.92%	6.776%
9	6.887	810	815	820	rBV	716588	882895	20.55%	2.179%
10	6.963	820	828	832	rBV	535905	659118	15.34%	1.626%
11	7.004	832	835	839	rVB	77211	88612	2.06%	0.219%
12	7.445	900	910	914	rBV	1406315	1967337	45.79%	4.854%
13	7.481	914	916	920	rVB	285346	316770	7.37%	0.782%
14	7.698	948	953	957	rBV	346966	435586	10.14%	1.075%
15	7.792	964	969	973	rBV	48578	72313	1.68%	0.178%
16	7.881	979	984	986	rBV2	177606	260187	6.06%	0.642%
17	7.916	986	990	995	rVB	851093	1073712	24.99%	2.649%
18	7.975	995	1000	1003	rBV	82231	111187	2.59%	0.274%
19	8.022	1003	1008	1012	rVB2	59935	95852	2.23%	0.237%
20	8.075	1012	1017	1020	rBV	290560	406599	9.46%	1.003%
21	8.110	1020	1023	1028	rVV2	345928	472284	10.99%	1.165%
22	8.169	1028	1033	1039	rVV	889890	1163647	27.08%	2.871%
23	8.222	1039	1042	1047	rVB2	36222	48177	1.12%	0.119%
24	8.298	1050	1055	1058	rBV	34323	44146	1.03%	0.109%
25	8.757	1129	1133	1136	rBV	51266	64310	1.50%	0.159%
26	8.875	1146	1153	1156	rBV2	37267	58009	1.35%	0.143%
27	9.092	1177	1190	1192	rBV9	20757	61155	1.42%	0.151%
28	9.245	1209	1216	1222	rBV	2000921	2651043	61.70%	6.541%
29	9.298	1222	1225	1227	rVV	43373	63701	1.48%	0.157%
30	9.322	1227	1229	1235	rVB	48004	57118	1.33%	0.141%
31	9.922	1324	1331	1345	rVB	981150	1273032	29.63%	3.141%
32	10.222	1377	1382	1392	rBV	18627	52231	1.22%	0.129%
33	10.633	1447	1452	1459	rBV	193504	247379	5.76%	0.610%
34	10.710	1459	1465	1475	rBV	1355466	1756791	40.89%	4.335%
35	10.828	1481	1485	1494	rVB	41628	68566	1.60%	0.169%
36	10.945	1501	1505	1509	rVB	35949	43358	1.01%	0.107%

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Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Sampling : 1

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Stop Thrs : 0

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Max Peaks: 100

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If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

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37	11.275	1557	1561	1571	rVB	59351	105622	2.46%	0.261%
38	11.410	1579	1584	1589	rBV	914179	1142739	26.60%	2.820%
39	11.510	1597	1601	1610	rBV	65345	95280	2.22%	0.235%
40	11.933	1668	1673	1682	rBV	408259	599654	13.96%	1.480%
41	12.110	1699	1703	1708	rBV2	27338	46701	1.09%	0.115%
42	12.398	1748	1752	1755	rBV2	40328	60135	1.40%	0.148%
43	12.639	1790	1793	1801	rVB2	35219	72477	1.69%	0.179%
44	12.716	1802	1806	1812	rBV	163183	247377	5.76%	0.610%
45	12.992	1847	1853	1863	rBV	1262285	1648330	38.36%	4.067%
46	13.221	1886	1892	1896	rBV	84859	145015	3.38%	0.358%
47	13.445	1926	1930	1933	rBV2	33815	56918	1.32%	0.140%
48	13.533	1941	1945	1948	rBV	192177	259209	6.03%	0.640%
49	13.686	1966	1971	1974	rBV	217147	294193	6.85%	0.726%
50	13.721	1974	1977	1981	rBV	147633	187581	4.37%	0.463%
51	13.845	1994	1998	2002	rBV	220153	282541	6.58%	0.697%
52	13.892	2002	2006	2012	rBV	384509	641279	14.93%	1.582%
53	14.027	2024	2029	2031	rBV	614456	953505	22.19%	2.353%
54	14.110	2039	2043	2052	rBV	200135	297625	6.93%	0.734%
55	14.210	2057	2060	2073	rVB2	94960	194987	4.54%	0.481%
56	14.333	2077	2081	2085	rBV	68043	84575	1.97%	0.209%
57	14.527	2109	2114	2120	rBV	406648	807285	18.79%	1.992%
58	14.733	2145	2149	2159	rBV	98784	191722	4.46%	0.473%
59	14.821	2161	2164	2168	rVV	44476	56908	1.32%	0.140%
60	14.968	2186	2189	2197	rVB2	47934	72686	1.69%	0.179%
61	15.168	2218	2223	2226	rBV	136457	223350	5.20%	0.551%
62	15.204	2226	2229	2234	rVB	105977	185225	4.31%	0.457%
63	15.527	2278	2284	2296	rVB	446241	762355	17.74%	1.881%
64	15.962	2353	2358	2361	rBV2	55242	101832	2.37%	0.251%
65	16.004	2361	2365	2370	rVB	93264	159013	3.70%	0.392%
66	16.068	2371	2376	2382	rBV2	45864	122762	2.86%	0.303%
67	16.127	2383	2386	2391	rVB	44651	72373	1.68%	0.179%
68	16.210	2396	2400	2404	rVB2	49085	74339	1.73%	0.183%
69	16.774	2490	2496	2501	rBV2	50787	109507	2.55%	0.270%
70	17.080	2543	2548	2554	rBV4	29779	65235	1.52%	0.161%
71	17.362	2592	2596	2605	rVB2	61999	133869	3.12%	0.330%
72	17.639	2636	2643	2650	rVB6	80507	269605	6.28%	0.665%
73	17.715	2651	2656	2675	rVB5	154622	466793	10.86%	1.152%
74	17.980	2693	2701	2718	rBV5	95330	395840	9.21%	0.977%
75	18.245	2735	2746	2763	rBV	580698	1764342	41.07%	4.354%

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ClientSampleId :
B-180-SB02

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Sum of corrected areas: 40526715

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Data File : BF140064.D
Acq On : 26 Oct 2024 17:16
Operator : RC/JU
Sample : P4471-02
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B-180-SB02

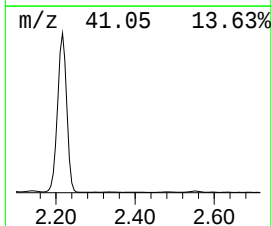
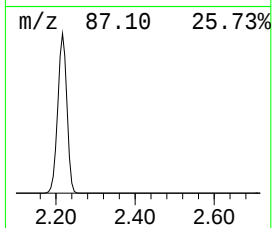
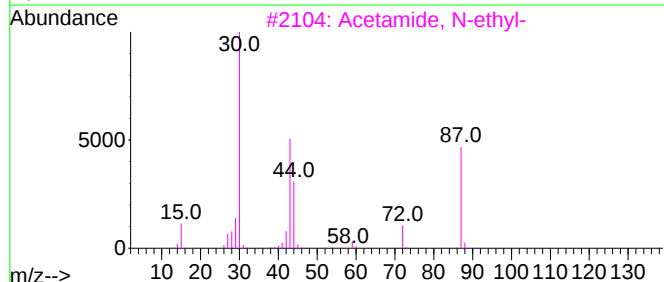
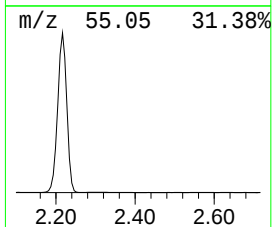
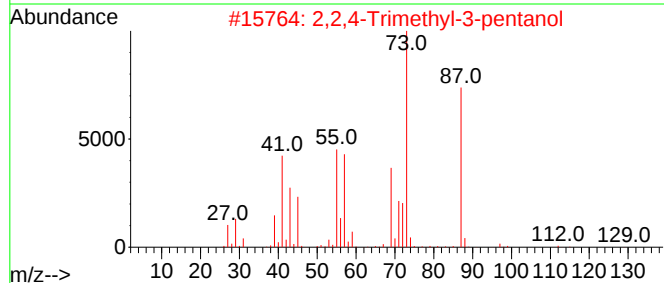
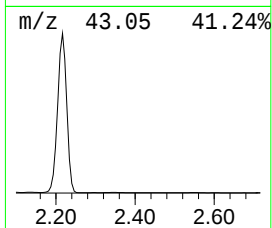
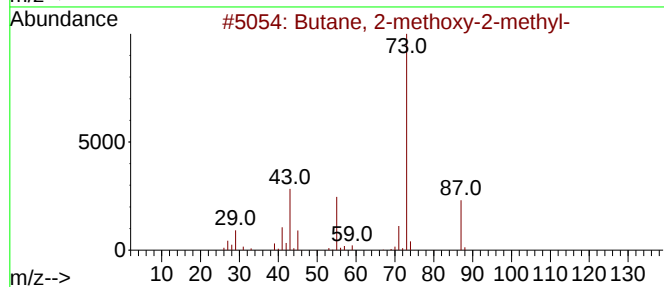
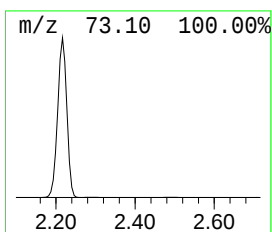
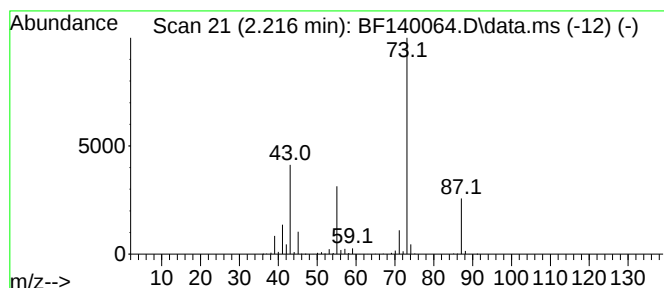
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.216	50.03 ng	2208510	1,4-Dichlorobenzene-d4	6.887

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	27
4			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
5			Octanal, 7-methoxy-3,7-dimethyl-	186	C11H22O2	003613-30-7	17



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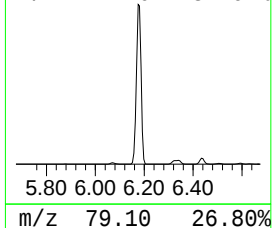
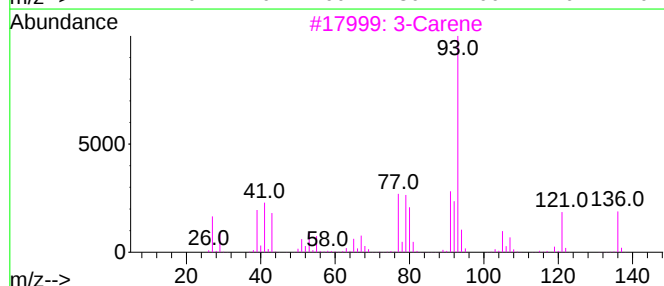
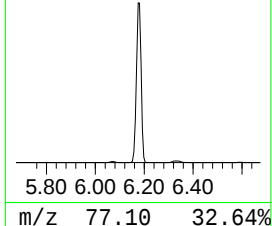
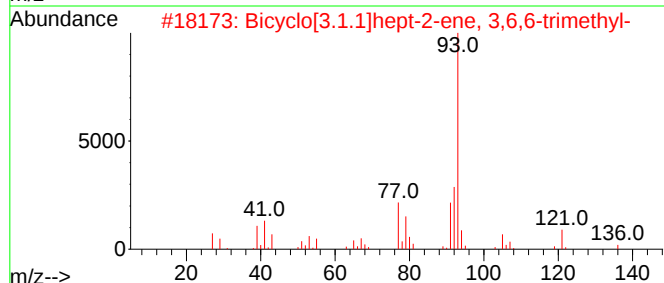
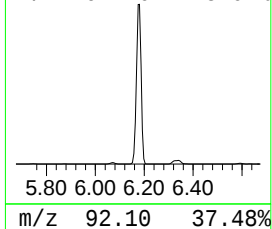
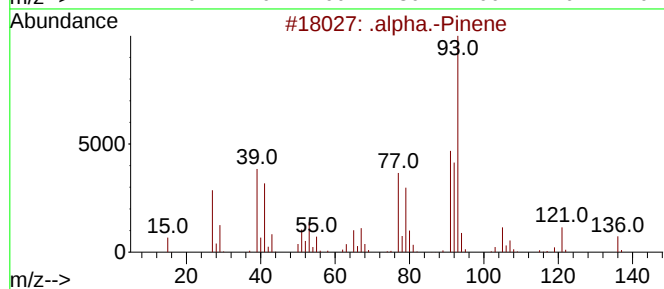
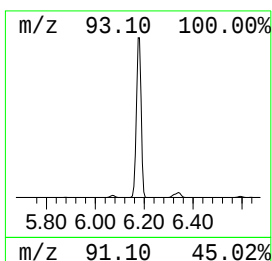
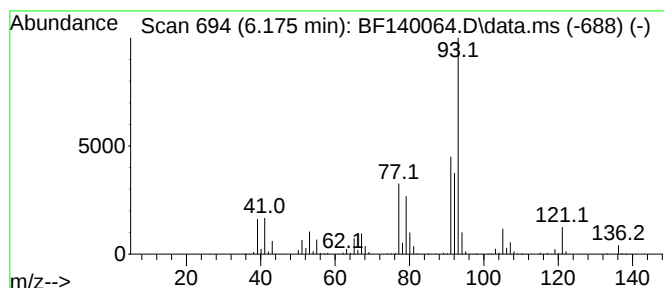
Instrument :
BNA_F
ClientSampleId :
B-180-SB02

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 .alpha.-Pinene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
6.175	97.33 ng	4296460	1,4-Dichlorobenzene-d4	6.887	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.alpha.-Pinene	136	C10H16	000080-56-8	94
2	Bicyclo[3.1.1]hept-2-ene, 3,6,6-...	136	C10H16	004889-83-2	91
3	3-Carene	136	C10H16	013466-78-9	91
4	Tricyclo[2.2.1.0(2,6)]heptane, 1...	136	C10H16	000508-32-7	91
5	(+)-3-Carene	136	C10H16	000498-15-7	91



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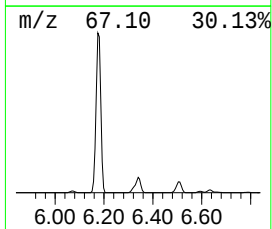
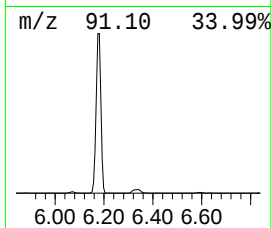
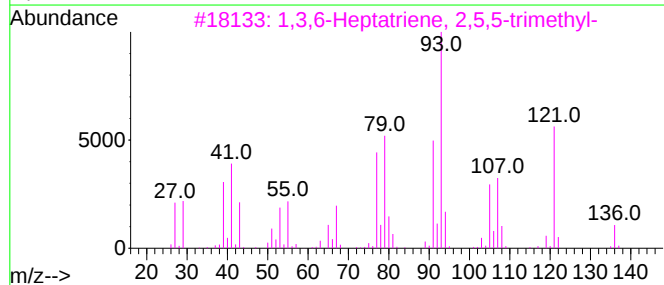
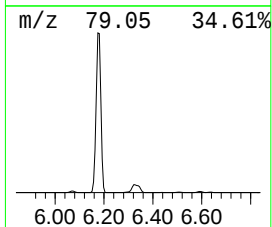
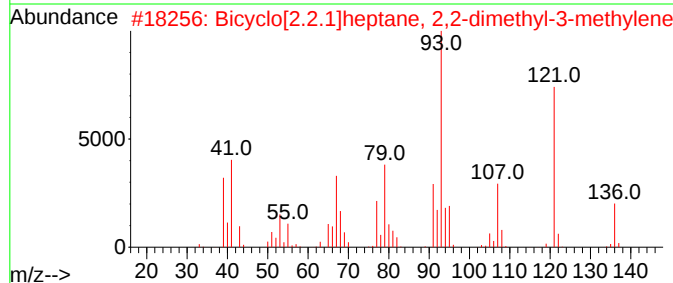
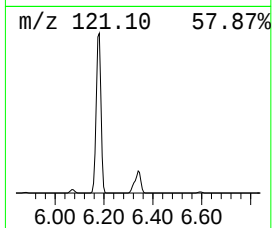
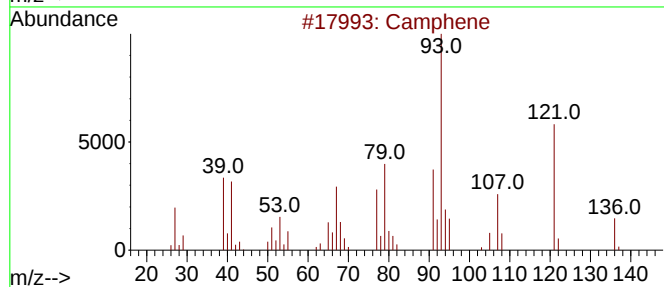
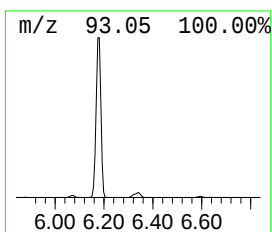
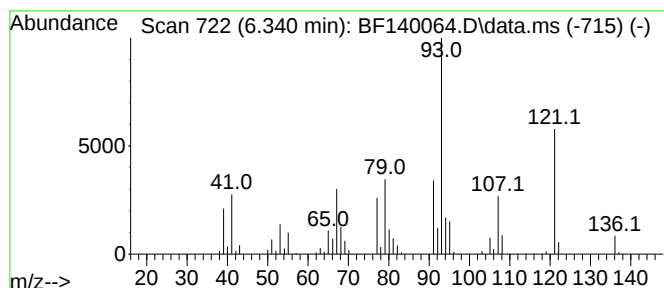
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Camphene Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.340	5.90 ng	260291	1,4-Dichlorobenzene-d4	6.887

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Camphene	136	C10H16	000079-92-5	95
2			Bicyclo[2.2.1]heptane, 2,2-dimet...	136	C10H16	005794-04-7	94
3			1,3,6-Heptatriene, 2,5,5-trimethyl-	136	C10H16	029548-02-5	90
4			Bicyclo[3.1.1]heptane, 6,6-dimet...	136	C10H16	018172-67-3	80
5			(+)-4-Carene	136	C10H16	029050-33-7	74



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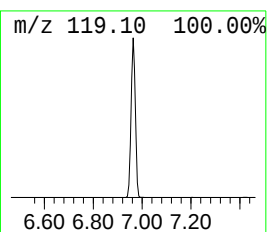
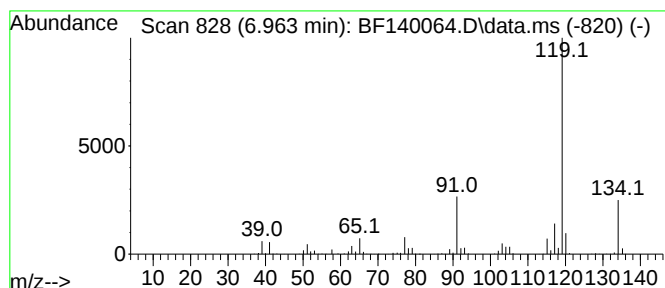
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

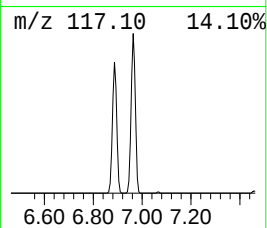
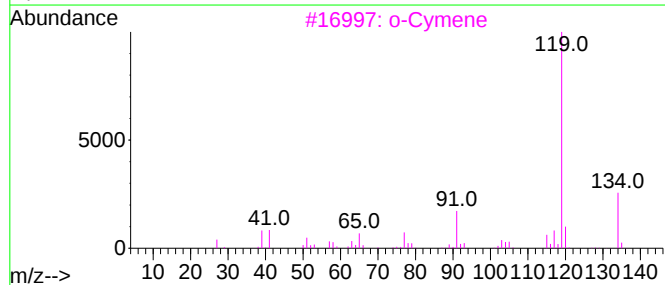
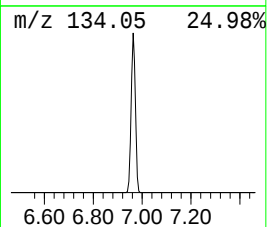
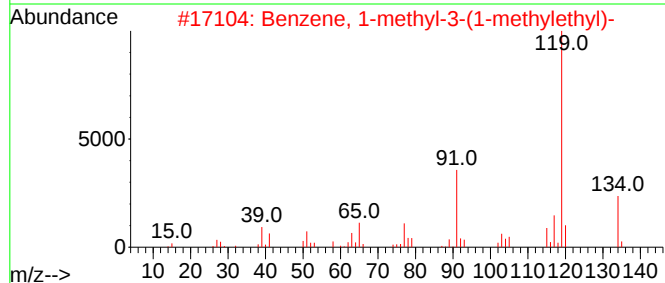
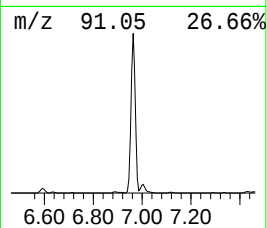
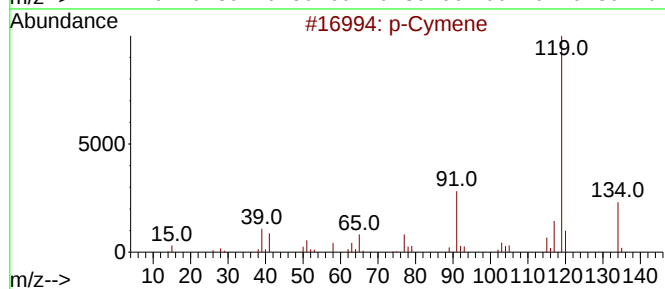
Peak Number 4 p-Cymene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.963	14.93 ng	659118	1,4-Dichlorobenzene-d4	6.887

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			p-Cymene	134	C10H14	000099-87-6	97
2			Benzene, 1-methyl-3-(1-methylethyl)-	134	C10H14	000535-77-3	95
3			o-Cymene	134	C10H14	000527-84-4	94
4			1,3,5-Cycloheptatriene, 3,7,7-trimethyl-	134	C10H14	003479-89-8	94
5			Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	91



m/z 91.05 26.66%



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Data File : BF140064.D
Acq On : 26 Oct 2024 17:16
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Sample : P4471-02
Misc :
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Instrument :
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ClientSampleId :
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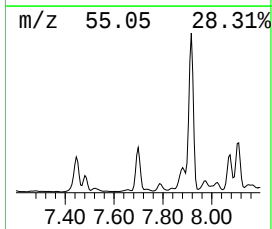
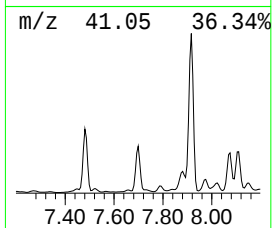
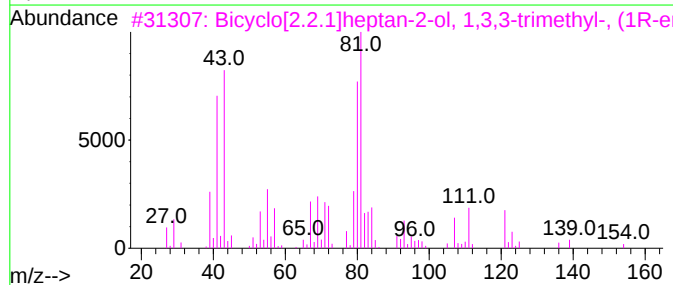
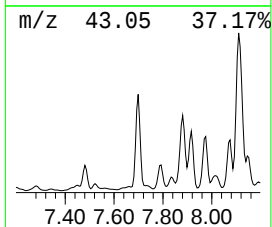
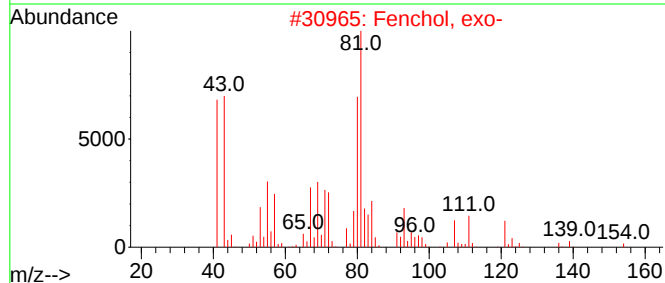
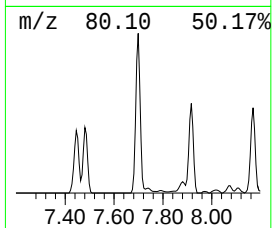
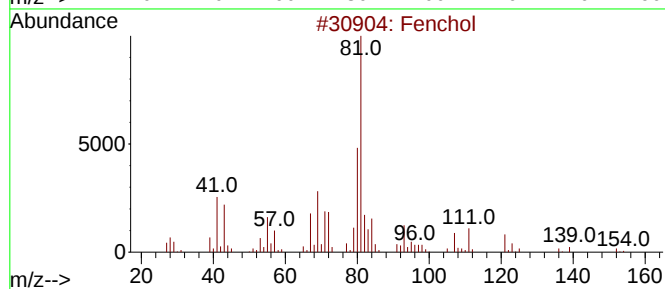
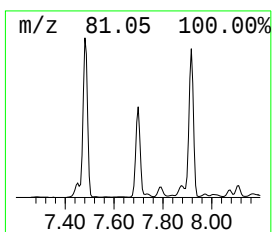
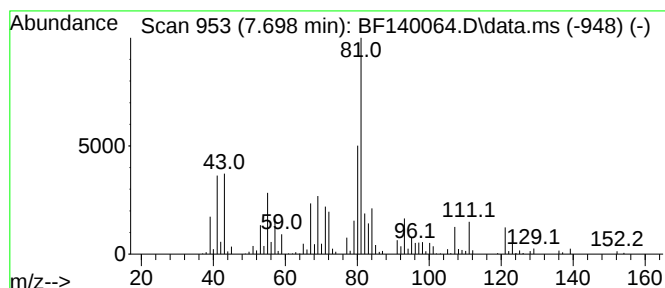
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Fenchol Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.698	7.49 ng	435586	Naphthalene-d8	8.169

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Fenchol	154	C10H18O	001632-73-1	96
2			Fenchol, exo-	154	C10H18O	022627-95-8	91
3			Bicyclo[2.2.1]heptan-2-ol, 1,3,3...	154	C10H18O	002217-02-9	38
4			Cyclohexane, 1,2-dichloro-	152	C6H10Cl2	001121-21-7	38
5			Cyclohexane, 1,2-dichloro-, trans-	152	C6H10Cl2	000822-86-6	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102624\
Data File : BF140064.D
Acq On : 26 Oct 2024 17:16
Operator : RC/JU
Sample : P4471-02
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B-180-SB02

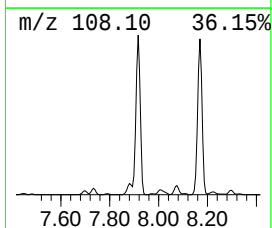
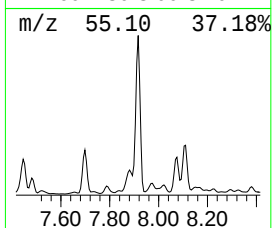
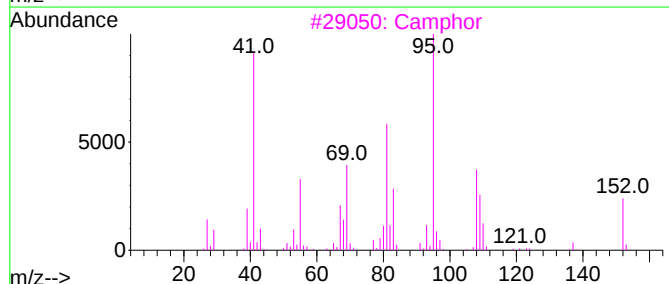
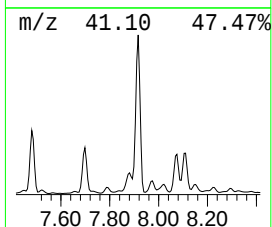
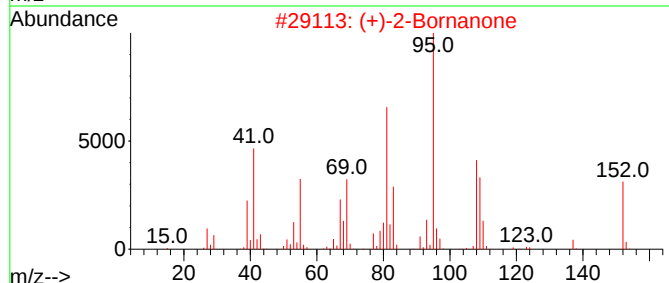
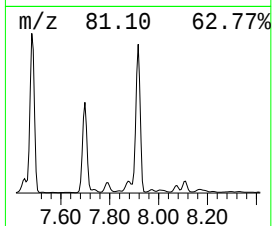
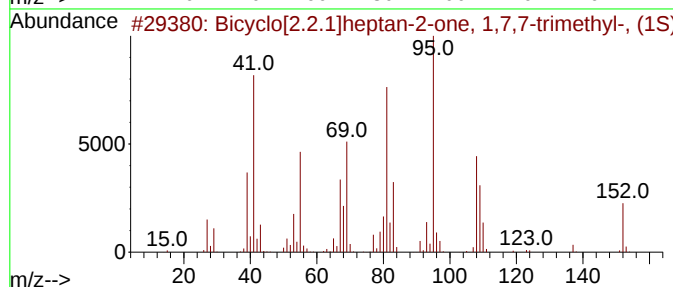
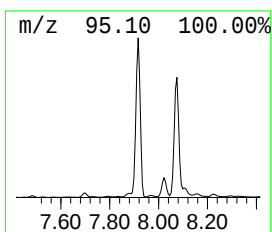
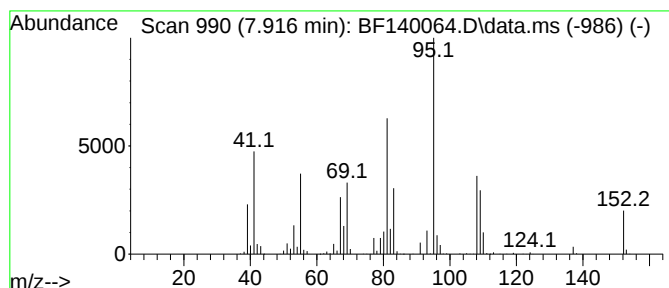
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Bicyclo[2.2.1]heptan-2-one,... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.916	18.45 ng	1073710	Naphthalene-d8	8.169

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Bicyclo[2.2.1]heptan-2-one, 1,7,...	152	C10H16O	000464-48-2	97
2		(+)-2-Bornanone	152	C10H16O	000464-49-3	97
3		Camphor	152	C10H16O	000076-22-2	97
4		5,7-Octadien-4-one, 2,6-dimethyl...	152	C10H16O	006752-80-3	58
5		1-Adamantanol	152	C10H16O	000768-95-6	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102624\
Data File : BF140064.D
Acq On : 26 Oct 2024 17:16
Operator : RC/JU
Sample : P4471-02
Misc :
ALS Vial : 16 Sample Multiplier: 1

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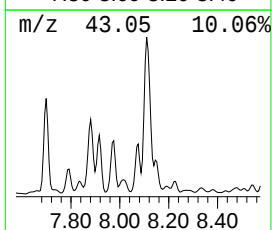
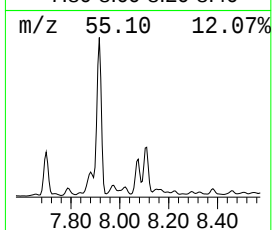
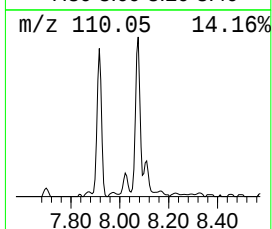
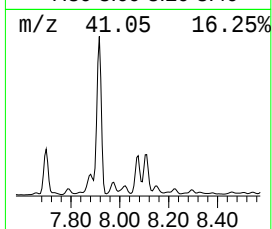
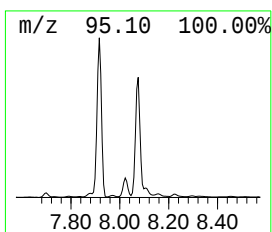
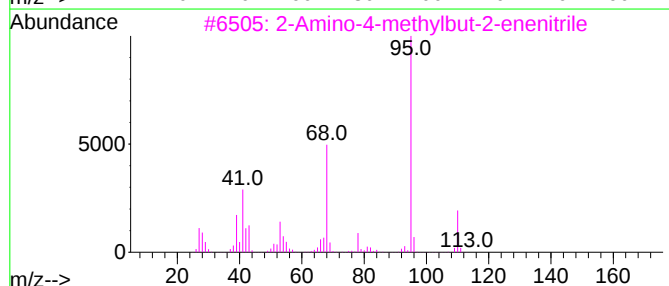
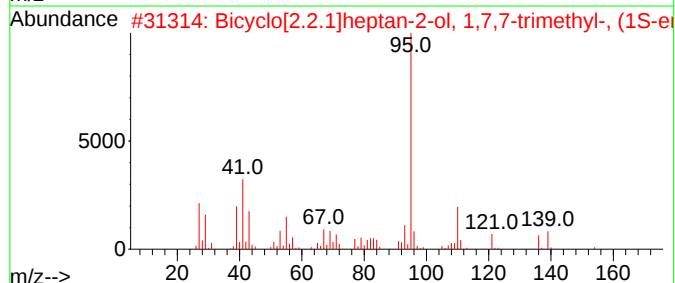
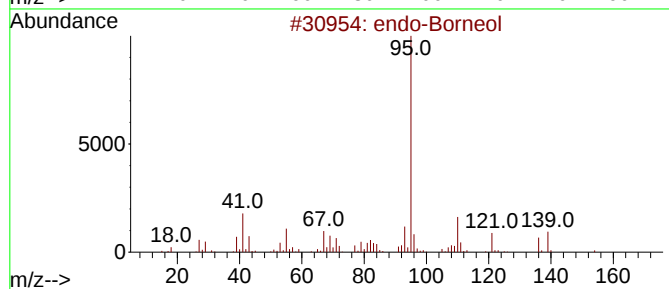
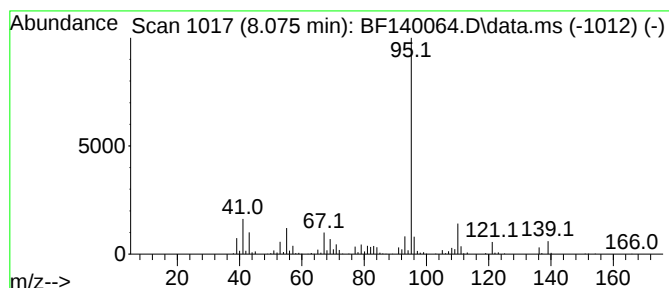
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 endo-Borneol Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.075	6.99 ng	406599	Naphthalene-d8	8.169

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			endo-Borneol	154	C10H18O	000507-70-0	91
2			Bicyclo[2.2.1]heptan-2-ol, 1,7,7...	154	C10H18O	000464-45-9	83
3			2-Amino-4-methylbut-2-enenitrile	110	C6H10N2	1000197-39-9	72
4			Bicyclo[2.2.1]heptane, 2-(1,1-di...	164	C12H20	069219-08-5	64
5			Furan, 2-ethyl-5-methyl-	110	C7H10O	001703-52-2	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102624\
Data File : BF140064.D
Acq On : 26 Oct 2024 17:16
Operator : RC/JU
Sample : P4471-02
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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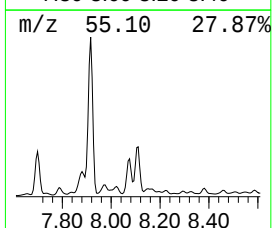
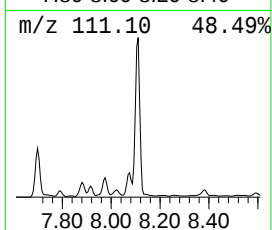
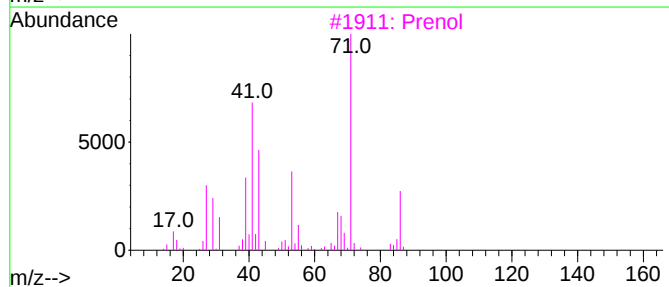
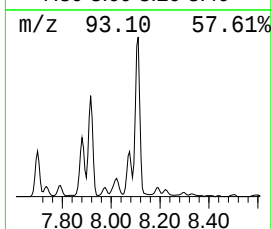
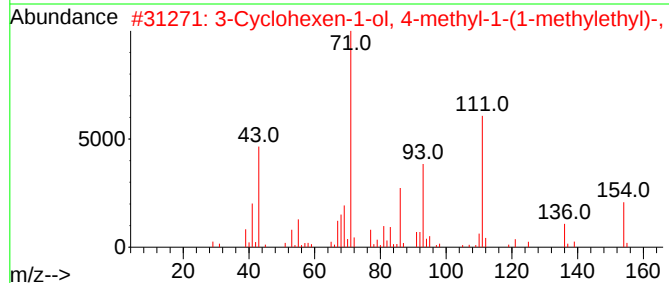
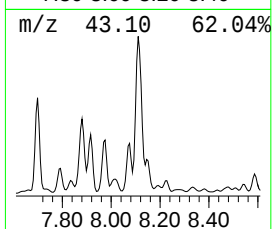
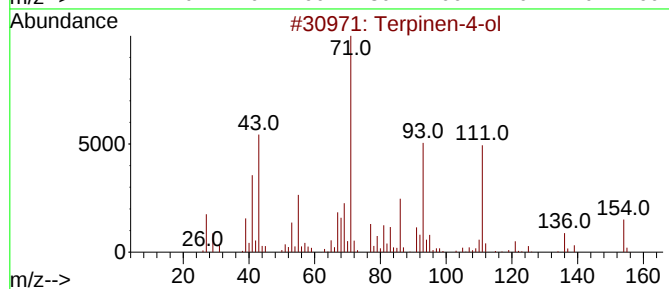
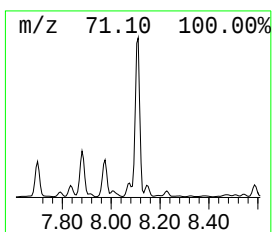
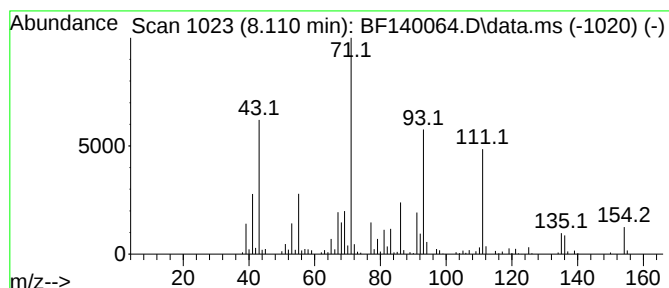
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 Terpinen-4-ol Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.110	8.12 ng	472284	Naphthalene-d8	8.169

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Terpinen-4-ol	154	C10H18O	000562-74-3	91
2		3-Cyclohexen-1-ol, 4-methyl-1-(1-methylethyl)-	154	C10H18O	020126-76-5	81
3		Prenol	86	C5H10O	000556-82-1	43
4		Bicyclo[3.1.1]heptan-endo-6-ol, ...	190	C7H11BrO	1000142-77-8	35
5		2-Butene, 1-methoxy-, (E)-	86	C5H10O	010034-14-7	30



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102624\
Data File : BF140064.D
Acq On : 26 Oct 2024 17:16
Operator : RC/JU
Sample : P4471-02
Misc :
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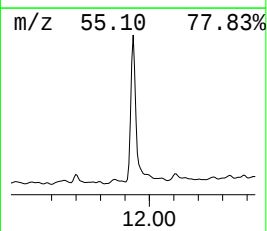
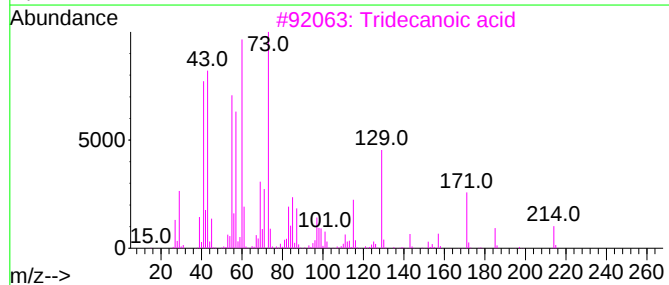
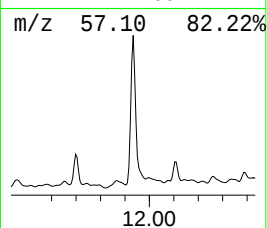
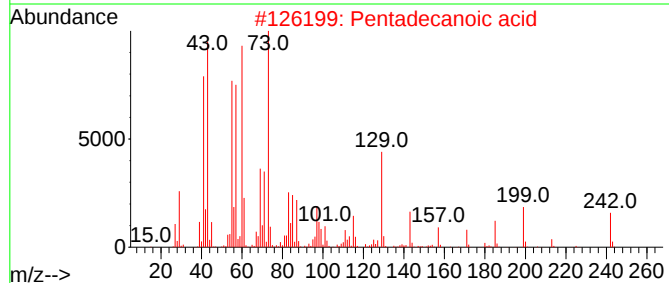
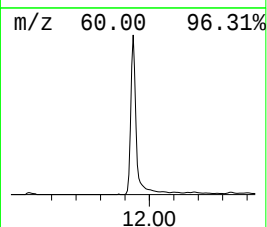
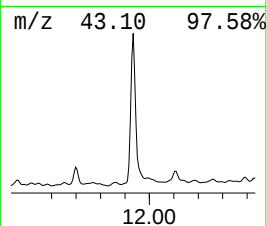
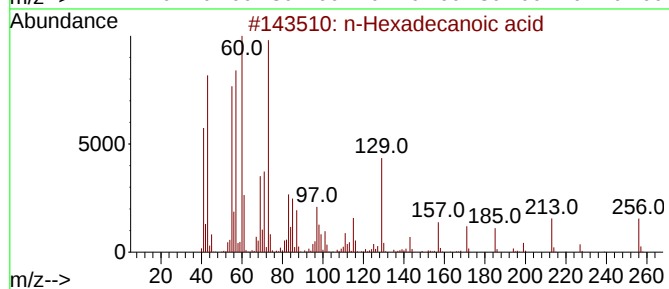
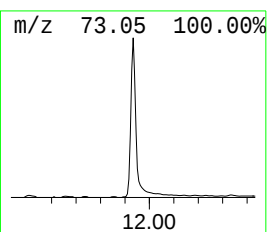
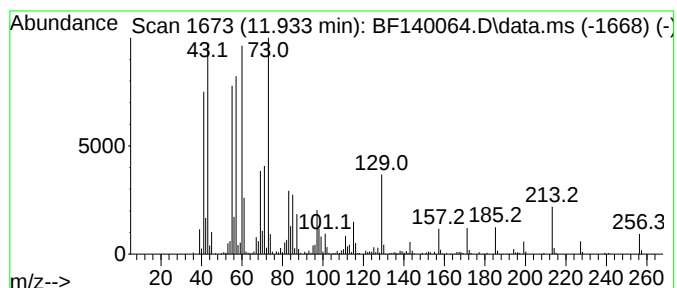
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 n-Hexadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.933	10.49 ng	599654	Phenanthrene-d10	11.410

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	91
3		Tridecanoic acid	214	C13H26O2	000638-53-9	89
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	83
5		Undecanoic acid	186	C11H22O2	000112-37-8	76



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102624\
Data File : BF140064.D
Acq On : 26 Oct 2024 17:16
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ClientSampleId :
B-180-SB02

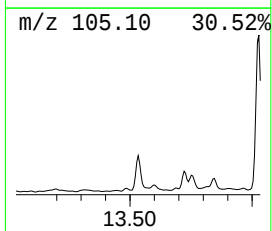
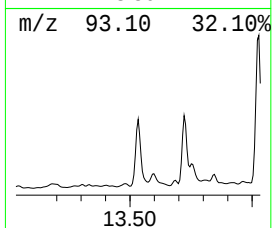
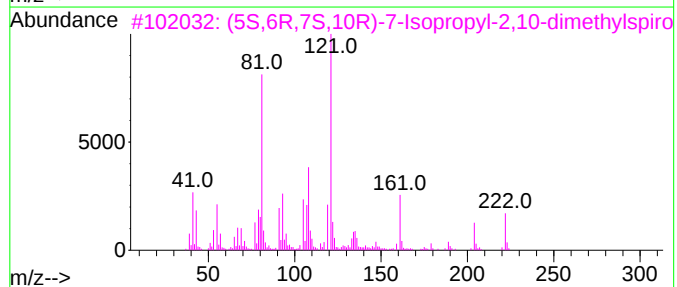
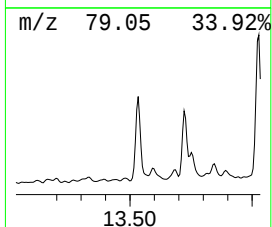
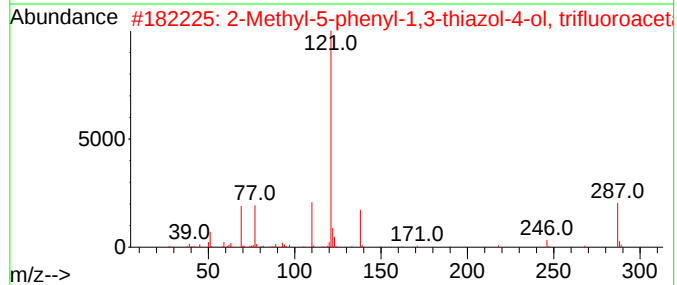
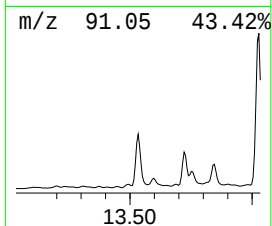
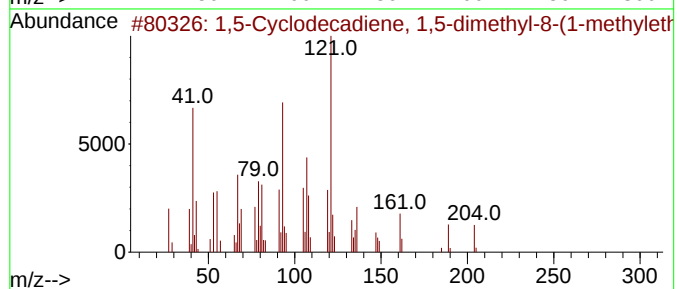
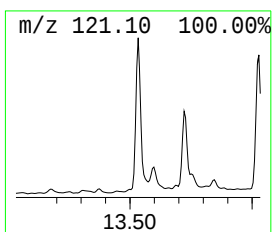
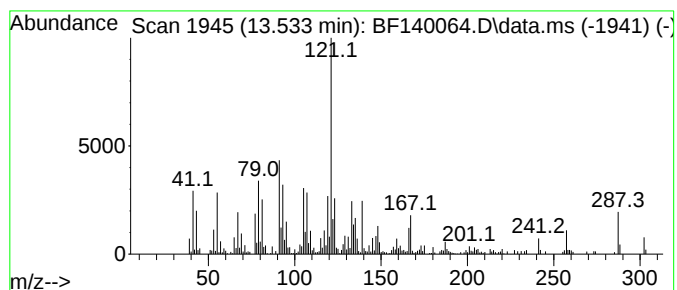
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 unknown13.533 Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.533	5.44 ng	259209	Chrysene-d12	14.045

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,5-Cyclodecadiene, 1,5-dimethyl...	204	C15H24	015423-57-1	47	
2	2-Methyl-5-phenyl-1,3-thiazol-4-...	287	C12H8F3N02S	1000471-95-1	43	
3	(5S,6R,7S,10R)-7-Isopropyl-2,10-...	222	C15H26O	072203-99-7	43	
4	.delta.8(14)-Isopimaric acid	302	C20H30O2	000471-74-9	42	
5	1,4-Cyclohexadiene, 3,3,6,6-tetr...	136	C10H16	002223-54-3	30	



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102624\
Data File : BF140064.D
Acq On : 26 Oct 2024 17:16
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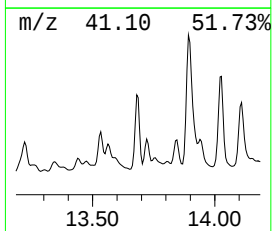
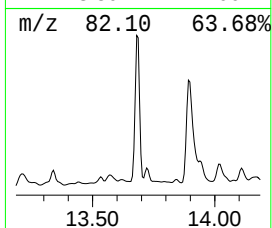
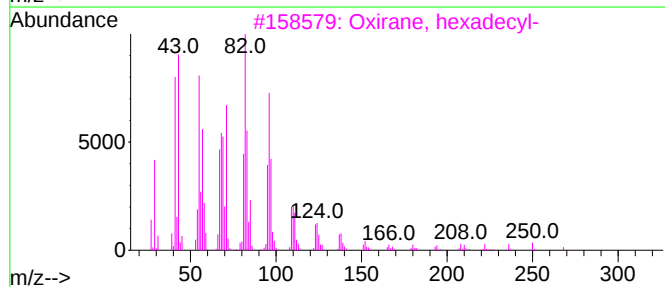
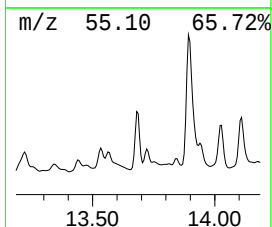
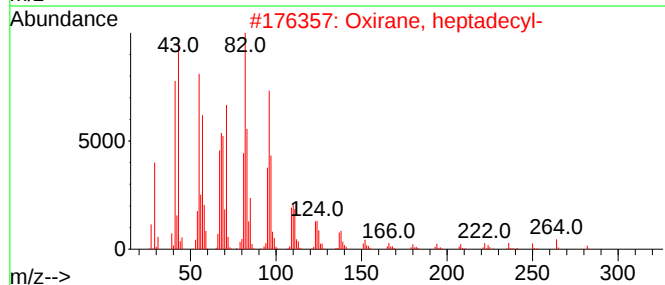
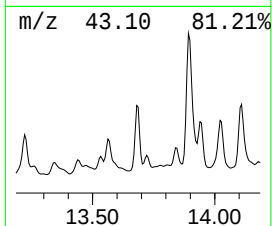
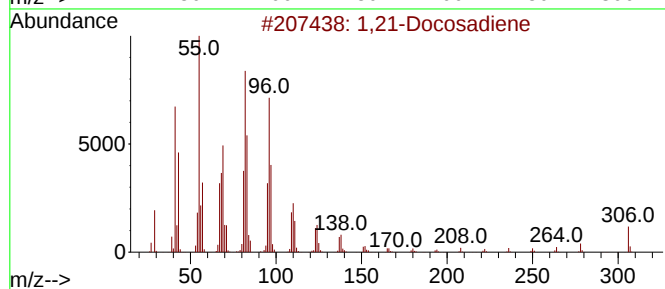
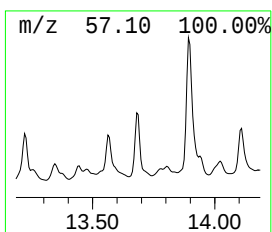
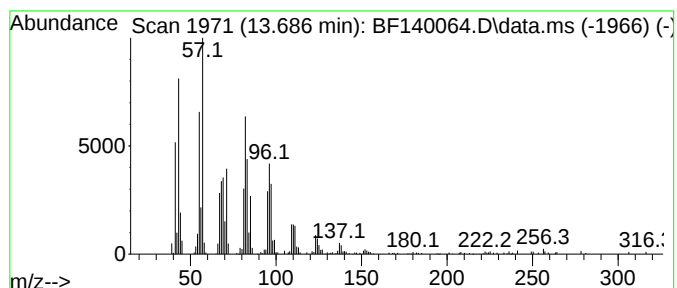
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 11 1,21-Docosadiene Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.686	6.17 ng	294193	Chrysene-d12	14.045

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,21-Docosadiene		306	C22H42	053057-53-7	96
2	Oxirane, heptadecyl-		282	C19H38O	067860-04-2	91
3	Oxirane, hexadecyl-		268	C18H36O	007390-81-0	91
4	Octadecanal		268	C18H36O	000638-66-4	91
5	Pentadecanal		226	C15H30O	002765-11-9	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102624\
Data File : BF140064.D
Acq On : 26 Oct 2024 17:16
Operator : RC/JU
Sample : P4471-02
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B-180-SB02

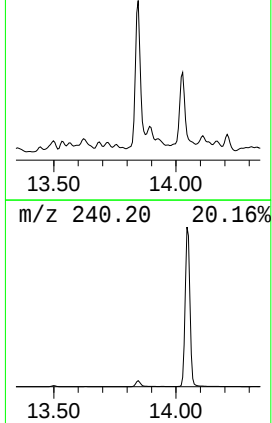
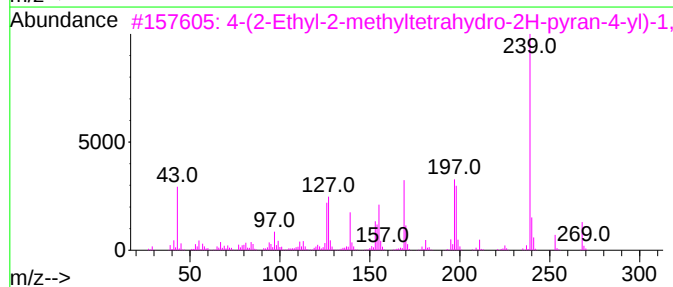
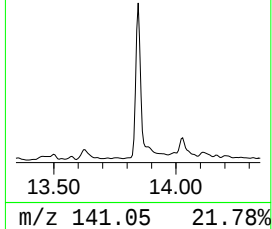
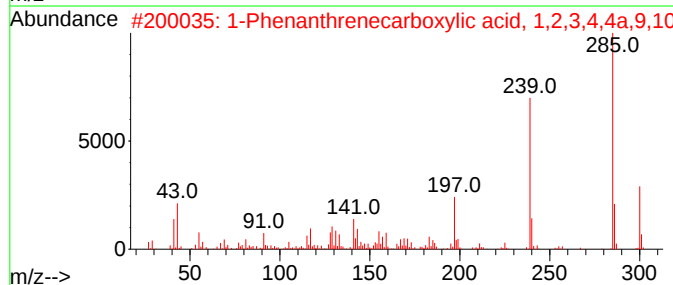
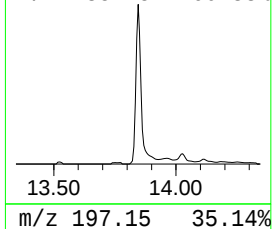
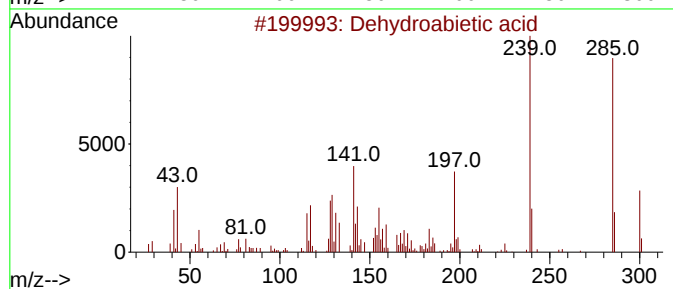
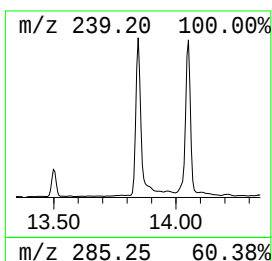
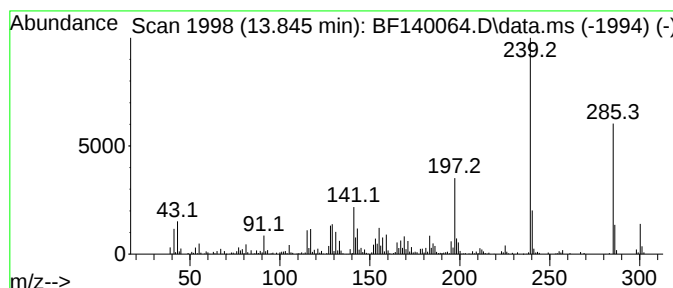
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 12 Dehydroabiatic acid Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.845	5.93 ng	282541	Chrysene-d12	14.045

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dehydroabiatic acid	300	C20H28O2	001740-19-8	99
2			1-Phenanthrenecarboxylic acid, 1...	300	C20H28O2	005155-70-4	94
3			4-(2-Ethyl-2-methyltetrahydro-2H...	268	C13H20N2O2S	1000479-90-5	43
4			2-Ethylidene-hydrazono-3-methyl...	239	C10H10C1N3S	1000148-08-4	43
5			Imidazolo[2,1-b]thiazole, 5-(3-i...	239	C13H9N3S	327097-37-0	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102624\
Data File : BF140064.D
Acq On : 26 Oct 2024 17:16
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Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B-180-SB02

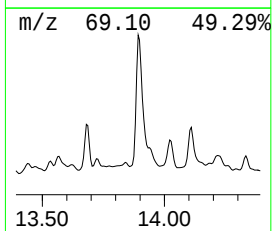
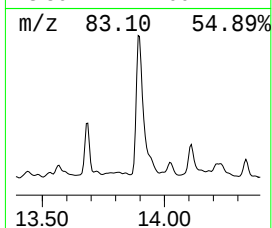
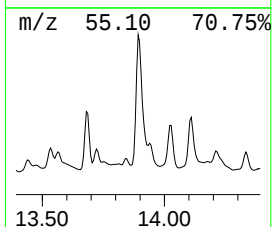
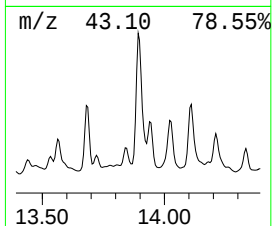
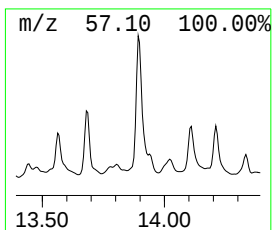
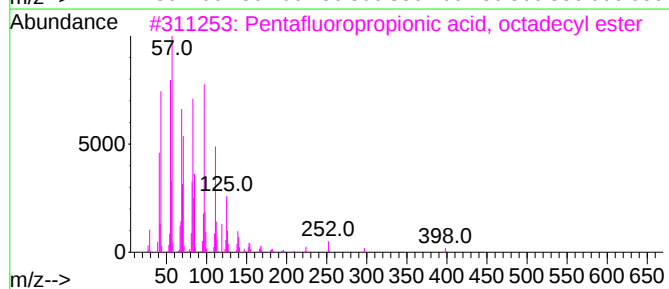
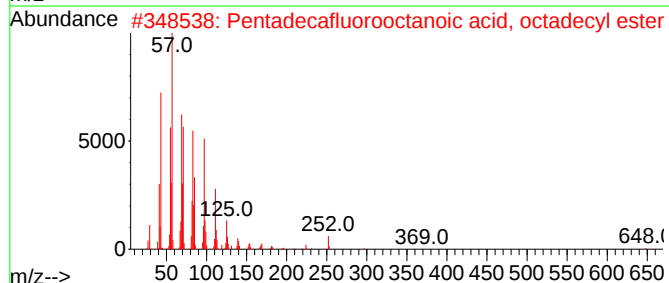
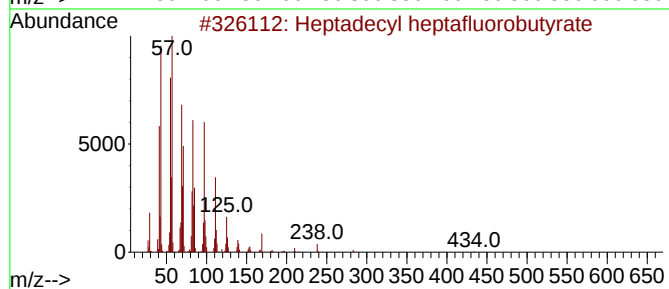
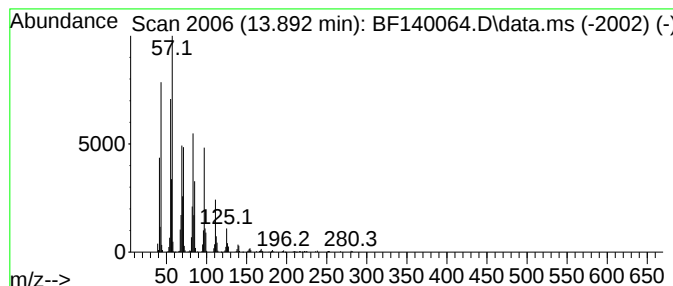
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 13 Heptadecyl heptafluorobutyrate Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.892	13.45 ng	641279	Chrysene-d12	14.045

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
2			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	94
3			Pentafluoropropionic acid, octad...	416	C21H37F5O2	959261-25-7	91
4			Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	91
5			Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102624\
Data File : BF140064.D
Acq On : 26 Oct 2024 17:16
Operator : RC/JU
Sample : P4471-02
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
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ClientSampleId :
B-180-SB02

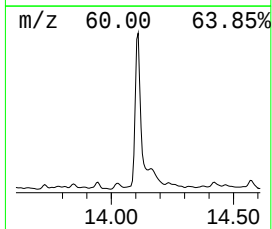
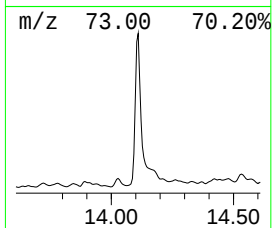
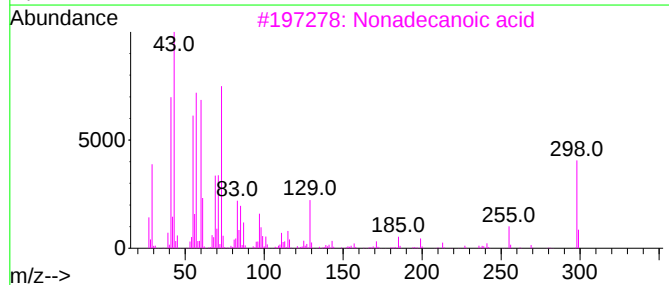
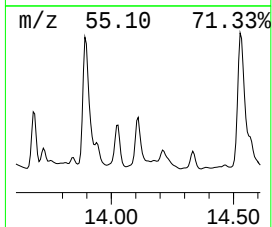
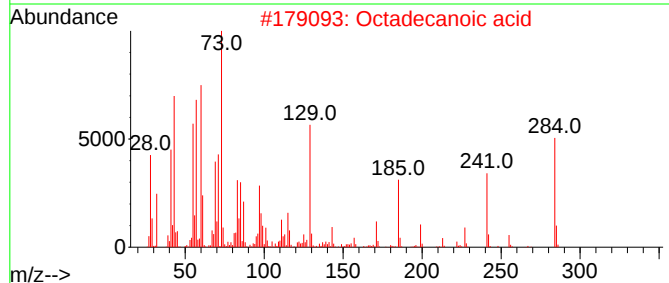
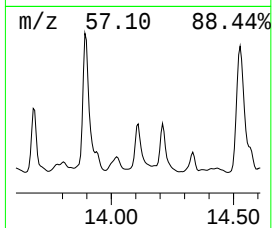
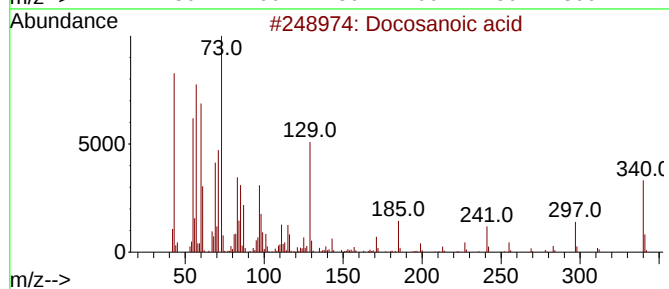
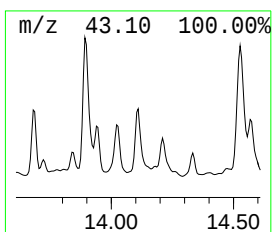
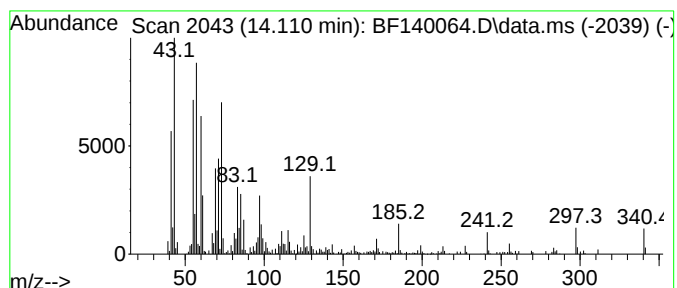
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 14 Docosanoic acid Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.110	6.24 ng	297625	Chrysene-d12	14.045

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Docosanoic acid	340	C22H44O2	000112-85-6	99
2		Octadecanoic acid	284	C18H36O2	000057-11-4	96
3		Nonadecanoic acid	298	C19H38O2	000646-30-0	95
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	60
5		Tridecanoic acid	214	C13H26O2	000638-53-9	45



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102624\
Data File : BF140064.D
Acq On : 26 Oct 2024 17:16
Operator : RC/JU
Sample : P4471-02
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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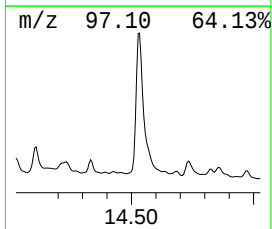
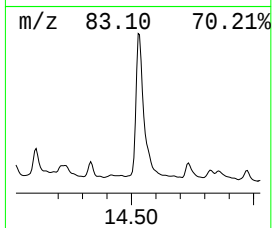
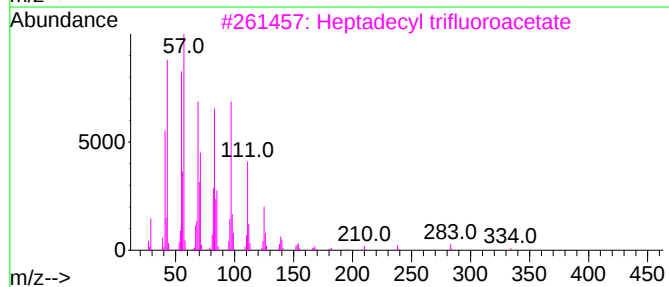
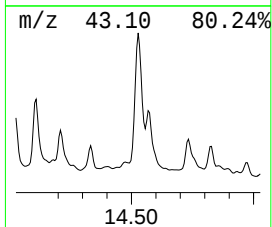
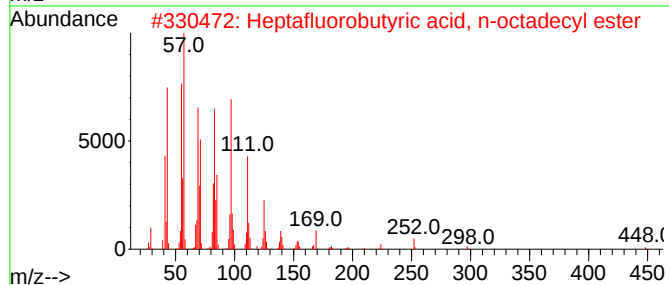
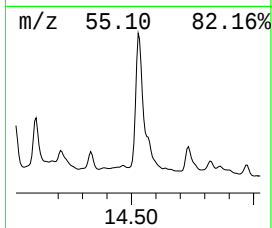
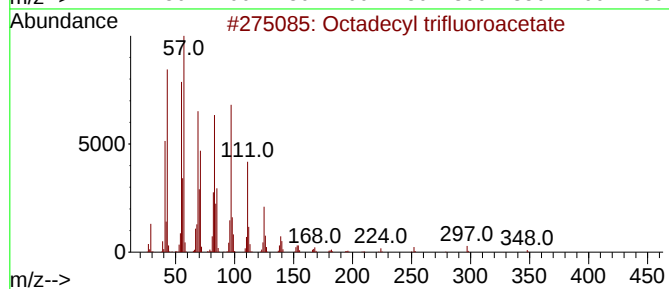
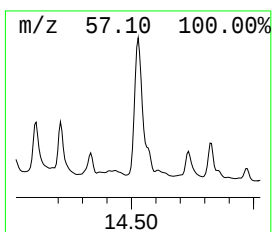
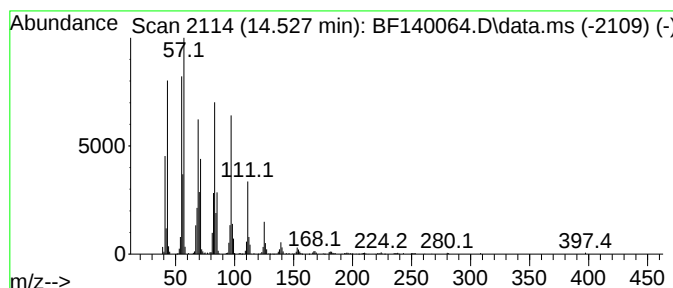
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 15 Octadecyl trifluoroacetate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.527	16.93 ng	807285	Chrysene-d12	14.045

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	94
2			Heptafluorobutyric acid, n-octadecyl ester	466	C22H37F7O2	000400-57-7	94
3			Heptadecyl trifluoroacetate	352	C19H35F3O2	1010351-87-0	94
4			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
5			Pentafluoropropionic acid, heptafluorobutyl ester	402	C20H35F5O2	959218-78-1	94



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102624\
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Acq On : 26 Oct 2024 17:16
Operator : RC/JU
Sample : P4471-02
Misc :
ALS Vial : 16 Sample Multiplier: 1

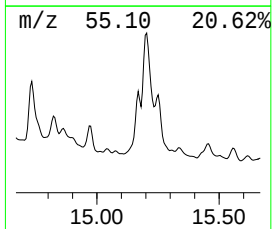
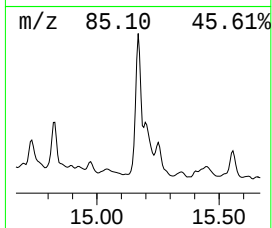
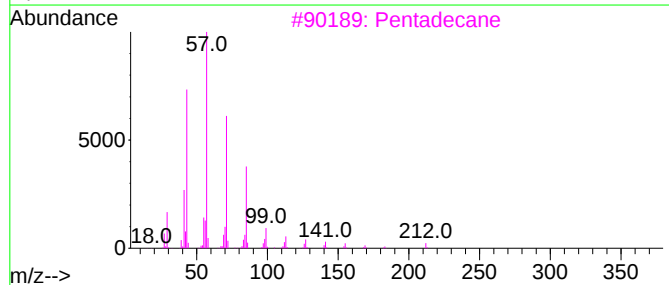
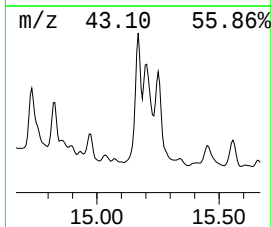
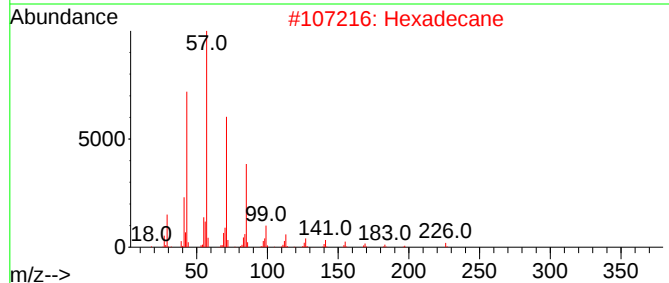
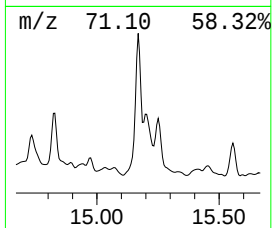
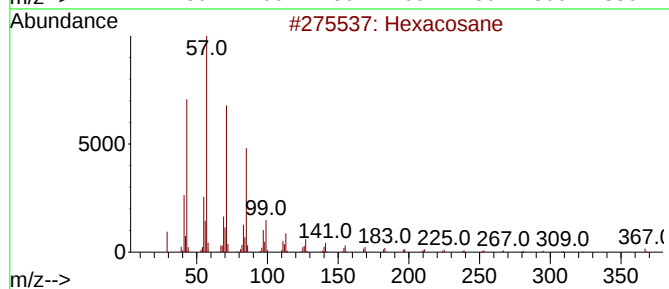
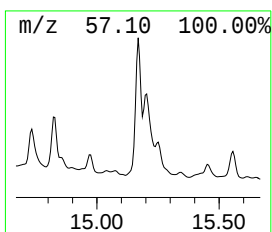
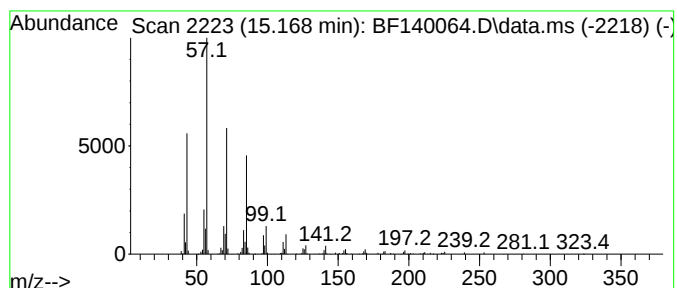
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 16 Hexacosane Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.168	5.86 ng	223350	Perylene-d12	15.527	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	94
2	Hexadecane	226	C16H34	000544-76-3	91
3	Pentadecane	212	C15H32	000629-62-9	90
4	Eicosane	282	C20H42	000112-95-8	87
5	Hexatriacontane	507	C36H74	000630-06-8	83



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102624\
Data File : BF140064.D
Acq On : 26 Oct 2024 17:16
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Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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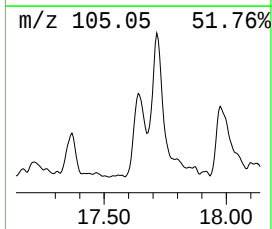
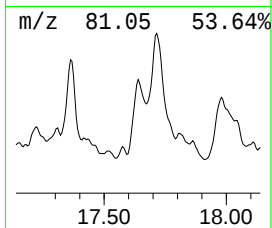
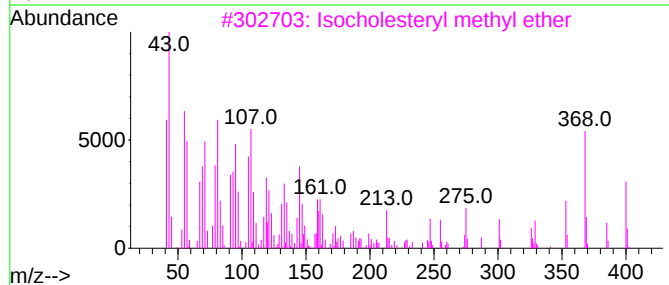
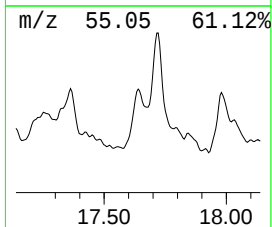
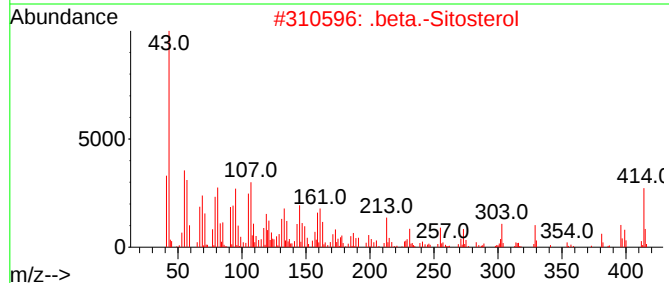
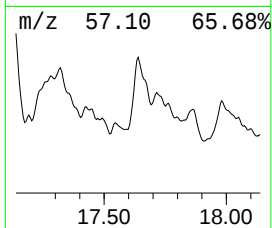
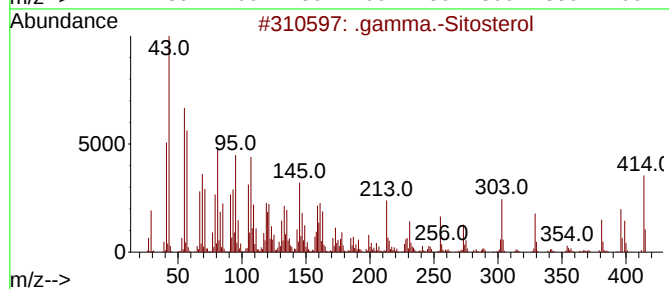
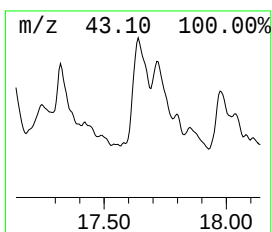
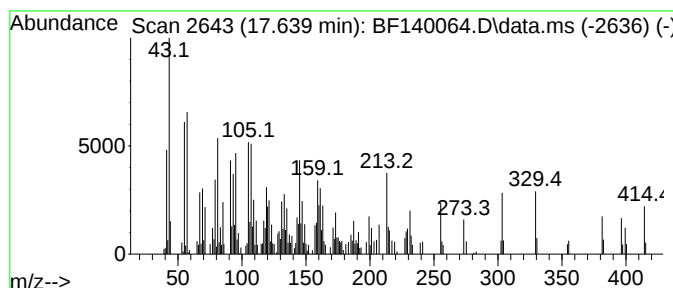
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 17 .gamma.-Sitosterol Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.639	7.07 ng	269605	Perylene-d12	15.527

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	.	gamma.-Sitosterol	414	C29H50O	000083-47-6	99	
2	.	beta.-Sitosterol	414	C29H50O	000083-46-5	97	
3	Isocholesteryl methyl ether	400	C28H48O	029944-53-4	53		
4	Campesterol	400	C28H48O	000474-62-4	49		
5	Ergost-5-en-3-ol, (3.beta.)-	400	C28H48O	004651-51-8	49		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102624\
Data File : BF140064.D
Acq On : 26 Oct 2024 17:16
Operator : RC/JU
Sample : P4471-02
Misc :
ALS Vial : 16 Sample Multiplier: 1

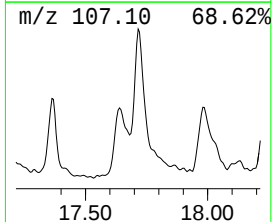
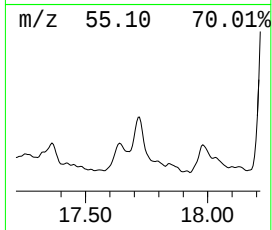
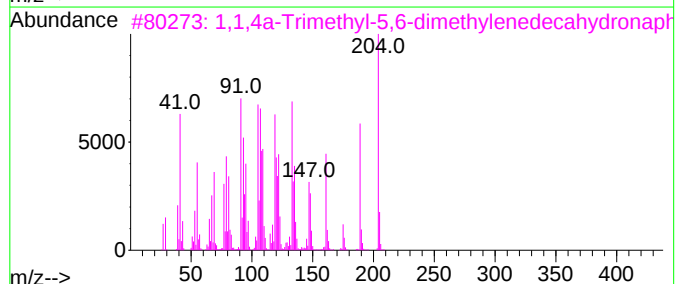
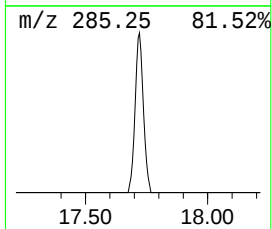
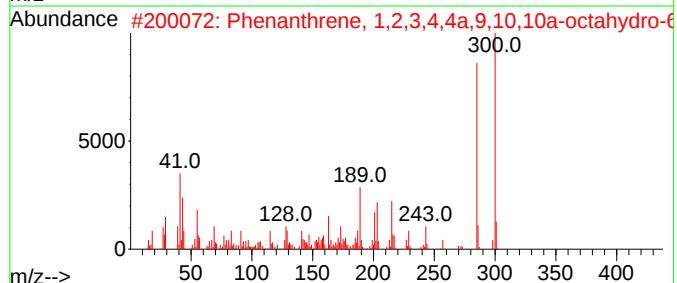
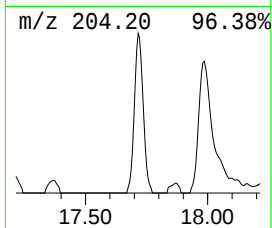
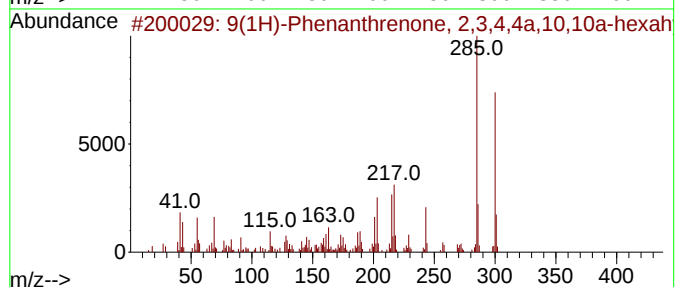
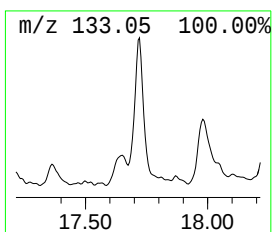
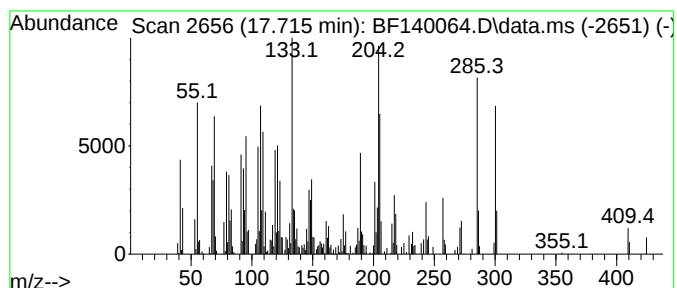
Instrument :
BNA_F
ClientSampleId :
B-180-SB02

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 18 9(1H)-Phenanthrenone, 2,3,4... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.		
17.715	12.25 ng	466793	Perylene-d12	15.527		
Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9(1H)-Phenanthrenone, 2,3,4,4a,1...	300	C20H28O2	000511-05-7	50	
2	Phenanthrene, 1,2,3,4,4a,9,10,10...	300	C21H32O	010064-26-3	35	
3	1,1,4a-Trimethyl-5,6-dimethylene...	204	C15H24	1000193-60-8	35	
4	2-(4-Fluorophenyl)-1,3-benzoxazo...	300	C16H17FN2OSi	1000479-98-9	30	
5	.beta.-Humulene	204	C15H24	000116-04-1	27	



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102624\
Data File : BF140064.D
Acq On : 26 Oct 2024 17:16
Operator : RC/JU
Sample : P4471-02
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B-180-SB02

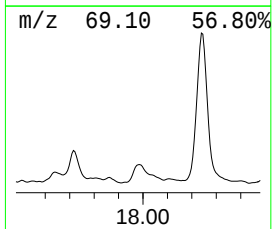
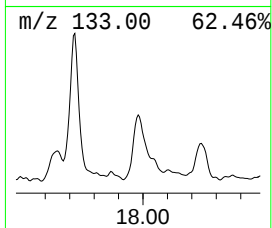
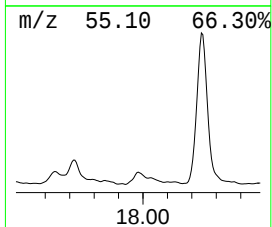
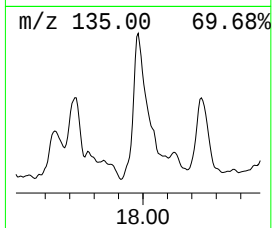
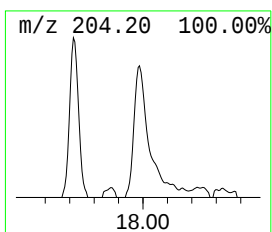
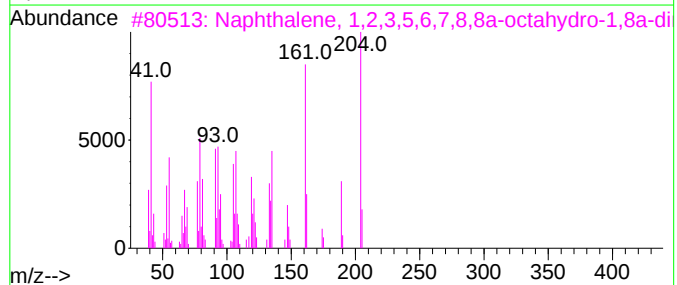
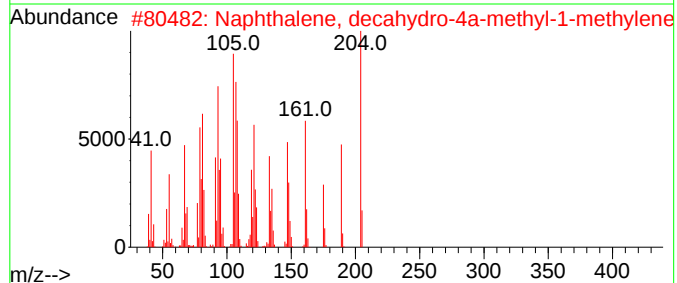
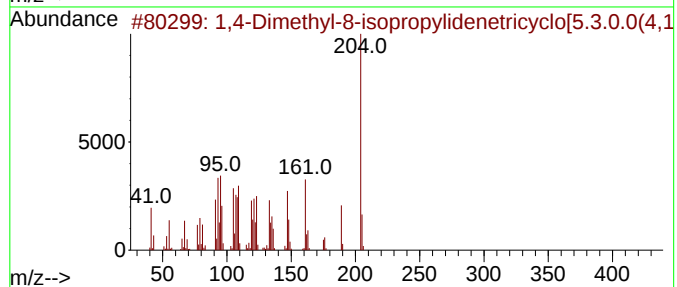
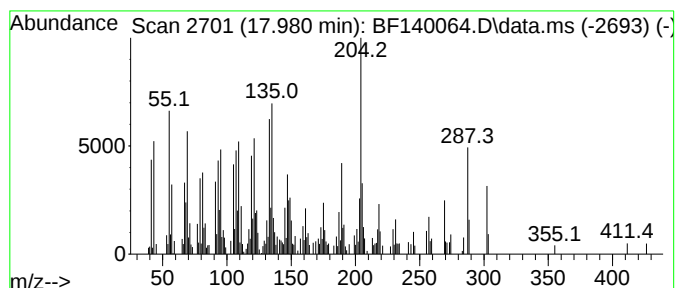
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 19 1,4-Dimethyl-8-isopropylide... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD		R.T.	
17.980	10.38 ng	395840	Perylene-d12		15.527	
Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1,4-Dimethyl-8-isopropylidenetri...	204	C15H24	1010140-07-7	70
2		Naphthalene, decahydro-4a-methyl...	204	C15H24	017066-67-0	70
3		Naphthalene, 1,2,3,5,6,7,8,8a-oc...	204	C15H24	004630-07-3	62
4		1,1,4a-Trimethyl-5,6-dimethylene...	204	C15H24	1000193-60-8	62
5		2,5,5,8a-Tetramethyl-6,7,8,8a-te...	204	C14H200	124957-09-1	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102624\
Data File : BF140064.D
Acq On : 26 Oct 2024 17:16
Operator : RC/JU
Sample : P4471-02
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B-180-SB02

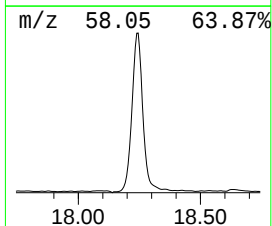
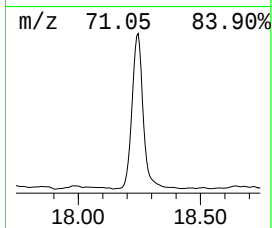
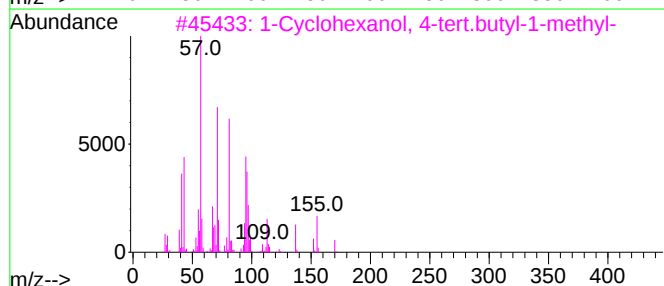
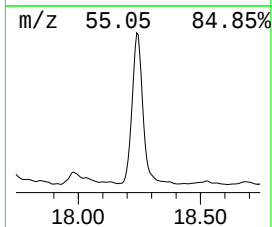
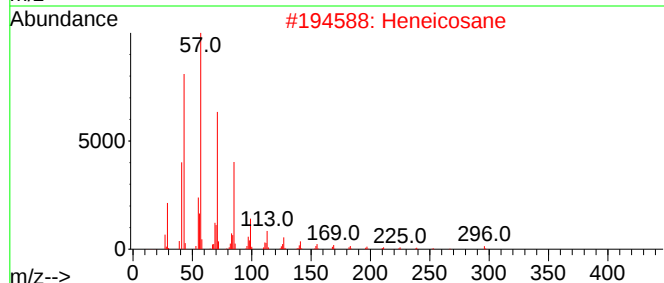
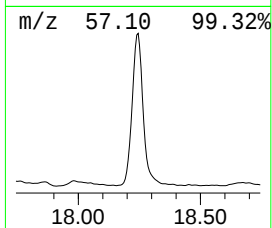
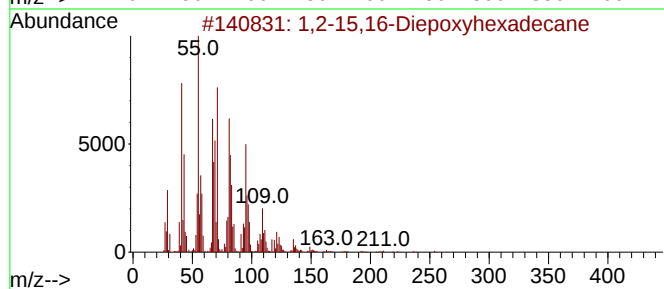
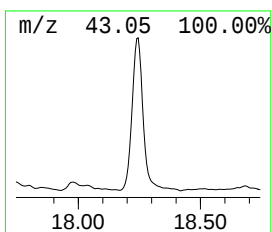
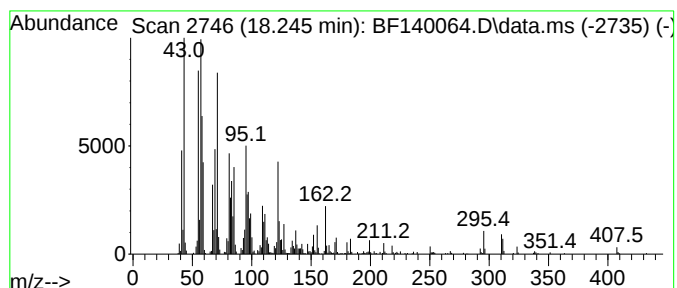
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 20 1,2-15,16-Diepoxyhexadecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.245	46.29 ng	1764340	Perylene-d12	15.527

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,2-15,16-Diepoxyhexadecane	254	C16H30O2	1000192-65-0	50	
2	Heneicosane	296	C21H44	000629-94-7	42	
3	1-Cyclohexanol, 4-tert.butyl-1-m...	170	C11H22O	1010163-45-0	42	
4	Tetradecane, 4-methyl-	212	C15H32	025117-24-2	38	
5	Carbonic acid, octadecyl prop-1-...	354	C22H42O3	1000383-11-5	30	



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102624\
Data File : BF140064.D
Acq On : 26 Oct 2024 17:16
Operator : RC/JU
Sample : P4471-02
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B-180-SB02

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.216	50.0	ng	2208510	1	6.887	882895	20.0
.alpha.-Pinene	6.175	97.3	ng	4296460	1	6.887	882895	20.0
Camphene	6.340	5.9	ng	260291	1	6.887	882895	20.0
p-Cymene	6.963	14.9	ng	659118	1	6.887	882895	20.0
Fenchol	7.698	7.5	ng	435586	2	8.169	1163650	20.0
Bicyclo[2.2.1]h...	7.916	18.4	ng	1073710	2	8.169	1163650	20.0
endo-Borneol	8.075	7.0	ng	406599	2	8.169	1163650	20.0
Terpinen-4-ol	8.110	8.1	ng	472284	2	8.169	1163650	20.0
n-Hexadecanoic ...	11.933	10.5	ng	599654	4	11.410	1142740	20.0
unknown13.533	13.533	5.4	ng	259209	5	14.045	953505	20.0
1,21-Docosadiene	13.686	6.2	ng	294193	5	14.045	953505	20.0
Dehydroabietic ...	13.845	5.9	ng	282541	5	14.045	953505	20.0
Heptadecyl hept...	13.892	13.4	ng	641279	5	14.045	953505	20.0
Docosanoic acid	14.110	6.2	ng	297625	5	14.045	953505	20.0
Octadecyl trifl...	14.527	16.9	ng	807285	5	14.045	953505	20.0
Hexacosane	15.168	5.9	ng	223350	6	15.527	762355	20.0
.gamma.-Sitosterol	17.639	7.1	ng	269605	6	15.527	762355	20.0
9(1H)-Phenanthr...	17.715	12.3	ng	466793	6	15.527	762355	20.0
1,4-Dimethyl-8-...	17.980	10.4	ng	395840	6	15.527	762355	20.0
1,2-15,16-Diepo...	18.245	46.3	ng	1764340	6	15.527	762355	20.0