

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102324\
 Data File : BF139983.D
 Acq On : 24 Oct 2024 00:11
 Operator : RC/JU
 Sample : P4385-14
 Misc :
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SP-7

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: BF139983.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.193	8	17	24	rVB	1419480	2261211	90.87%	9.422%
2	5.110	506	513	524	rVB	115941	174517	7.01%	0.727%
3	5.504	574	580	585	rBV	1860324	2407882	96.76%	10.033%
4	6.504	744	750	770	rVB	1754366	2333752	93.78%	9.724%
5	6.893	810	816	821	rVB	587285	750253	30.15%	3.126%
6	7.445	904	910	915	rBV	1195475	1509849	60.68%	6.291%
7	7.698	949	953	959	rVB	54241	64773	2.60%	0.270%
8	8.169	1028	1033	1038	rBV	736534	908261	36.50%	3.784%
9	8.381	1063	1069	1078	rVB2	21355	29942	1.20%	0.125%
10	9.245	1210	1216	1226	rBV	1952605	2488408	100.00%	10.368%
11	9.922	1325	1331	1336	rBV	660558	870790	34.99%	3.628%
12	9.957	1336	1337	1344	rVB2	35019	36133	1.45%	0.151%
13	10.634	1447	1452	1459	rBV	106759	133778	5.38%	0.557%
14	10.710	1459	1465	1475	rBV	940501	1208946	48.58%	5.037%
15	11.410	1579	1584	1591	rBV	638522	821629	33.02%	3.423%
16	11.933	1664	1673	1685	rBV	320669	511880	20.57%	2.133%
17	12.022	1686	1688	1697	rVB	15219	31362	1.26%	0.131%
18	12.622	1785	1790	1793	rBV	101345	155188	6.24%	0.647%
19	12.722	1802	1807	1814	rBV	73170	119231	4.79%	0.497%
20	12.780	1814	1817	1821	rVV3	29393	40510	1.63%	0.169%
21	12.851	1824	1829	1835	rVV	65069	95938	3.86%	0.400%
22	12.998	1848	1854	1860	rVB	1780302	2353796	94.59%	9.807%
23	13.063	1860	1865	1870	rBV5	12828	26241	1.05%	0.109%
24	13.227	1889	1893	1898	rBV2	23434	41330	1.66%	0.172%
25	13.445	1926	1930	1932	rBV4	20025	31136	1.25%	0.130%
26	13.569	1948	1951	1955	rBV	21553	30064	1.21%	0.125%
27	13.657	1963	1966	1969	rBV4	21380	34442	1.38%	0.144%
28	13.904	2003	2008	2018	rBV2	134502	291649	11.72%	1.215%
29	14.051	2025	2033	2045	rBV	675742	1027512	41.29%	4.281%
30	14.216	2058	2061	2066	rVB2	25232	31070	1.25%	0.129%
31	14.522	2109	2113	2116	rBV	66976	100953	4.06%	0.421%
32	15.174	2219	2224	2229	rBV	219567	328069	13.18%	1.367%
33	15.527	2279	2284	2296	rVB	408574	700705	28.16%	2.920%
34	15.774	2321	2326	2334	rVB	155229	251901	10.12%	1.050%
35	16.010	2361	2366	2373	rBV	159995	285153	11.46%	1.188%
36	16.833	2500	2506	2521	rVB	162529	356891	14.34%	1.487%

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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

37	17.398	2594	2602	2610	rVB	502538	1155057	46.42%	4.813%
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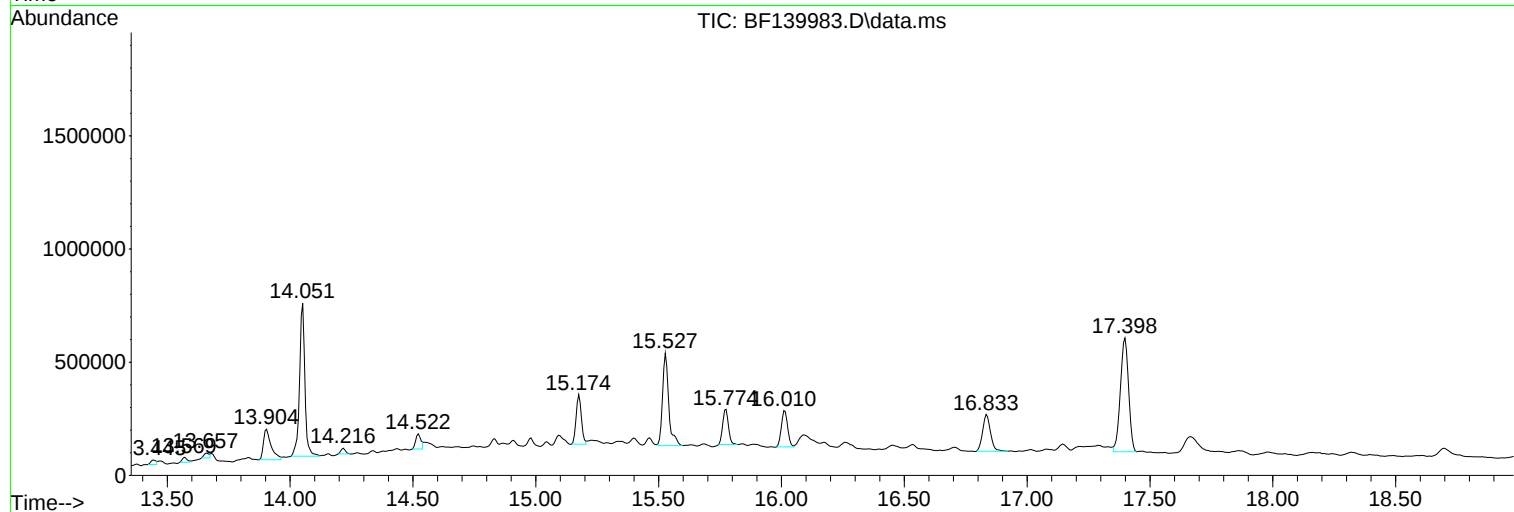
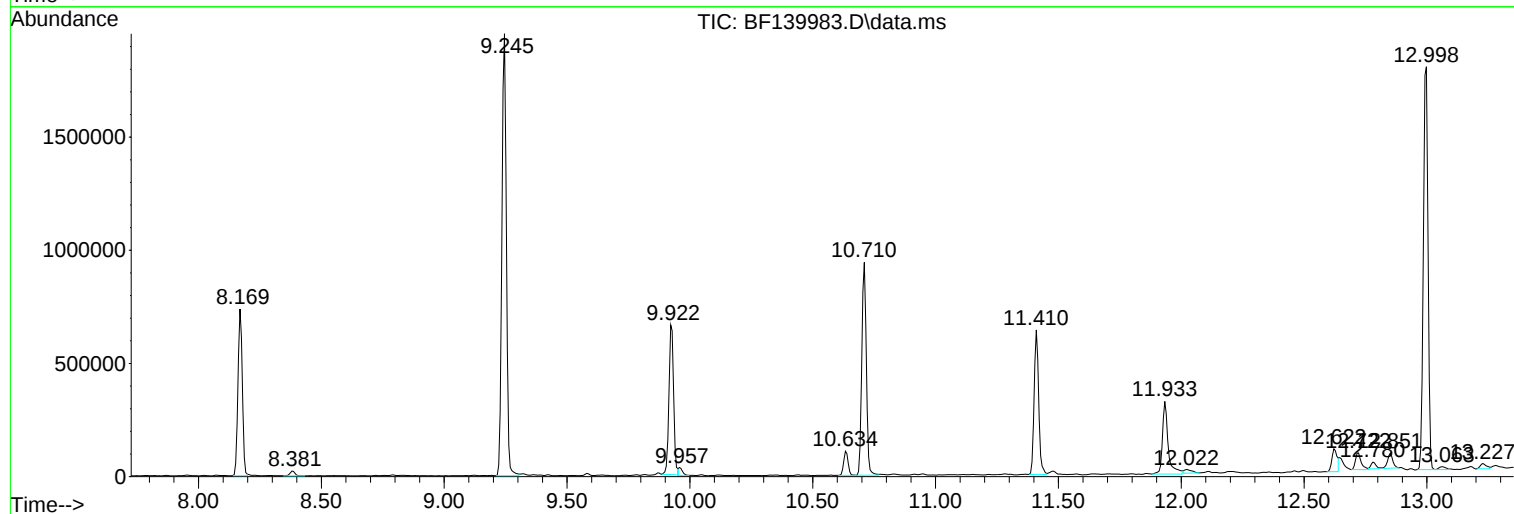
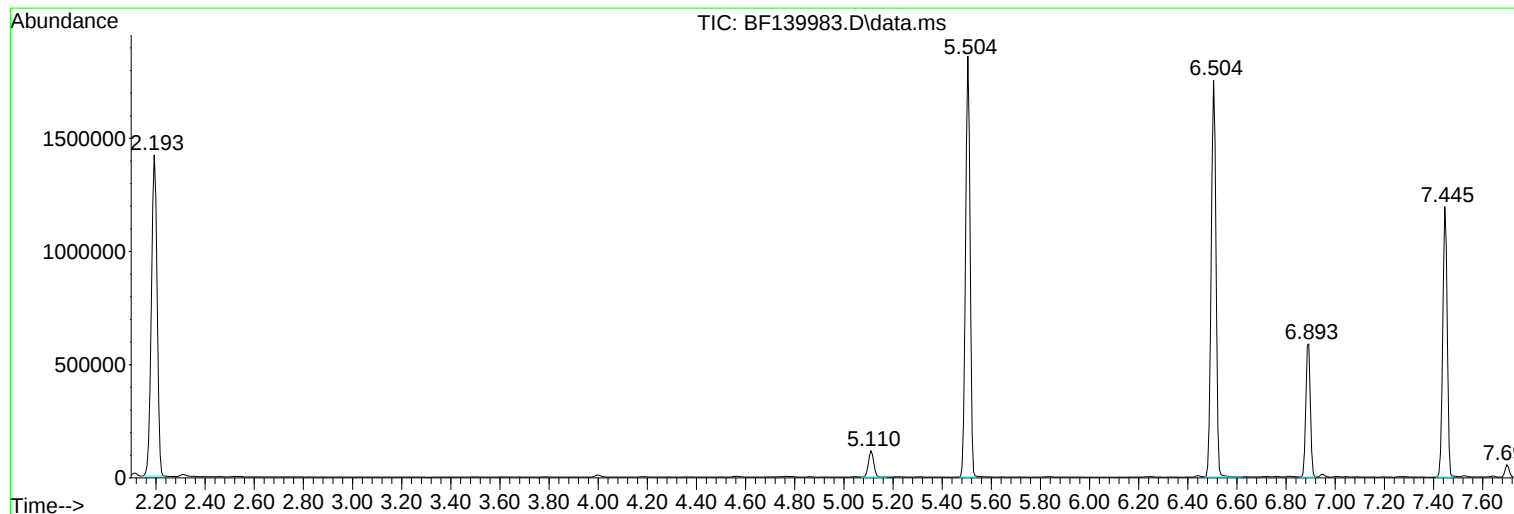
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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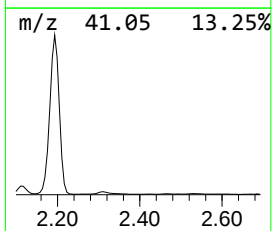
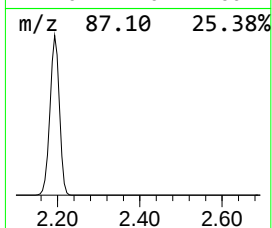
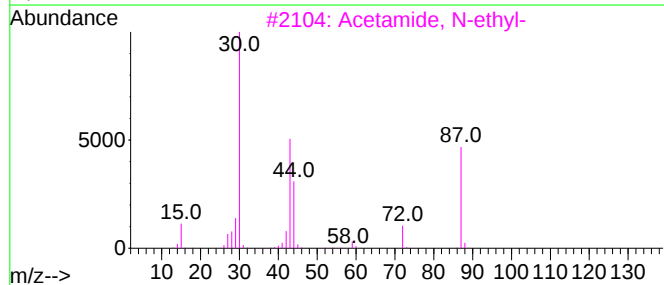
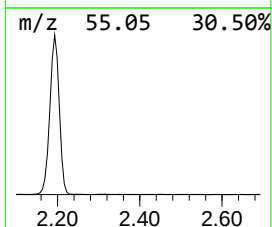
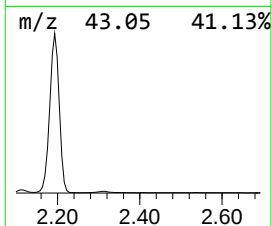
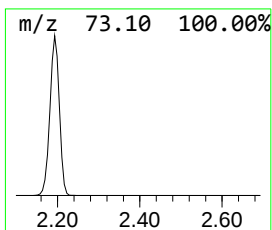
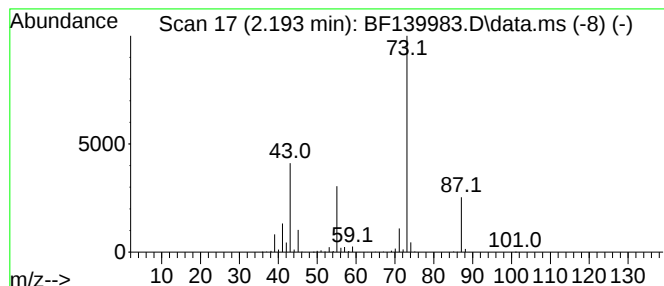
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.193	60.28 ng	2261210	1,4-Dichlorobenzene-d4	6.893

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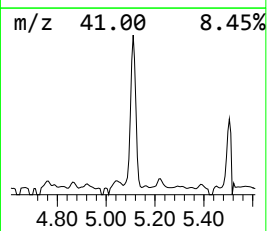
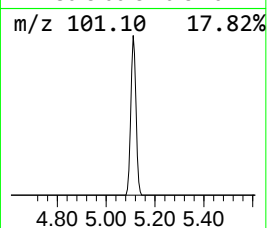
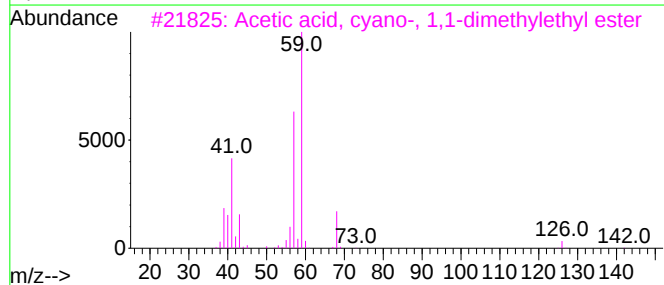
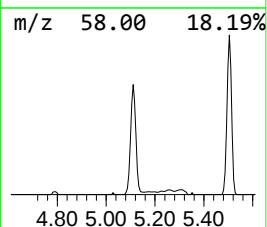
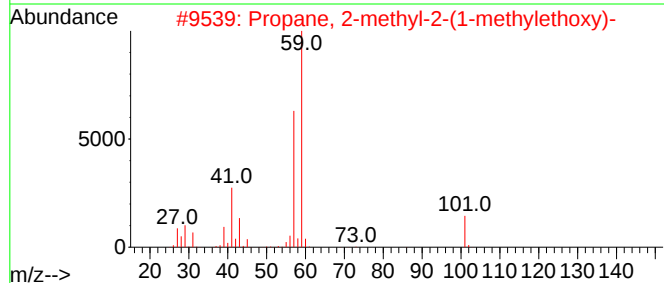
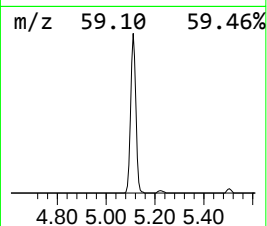
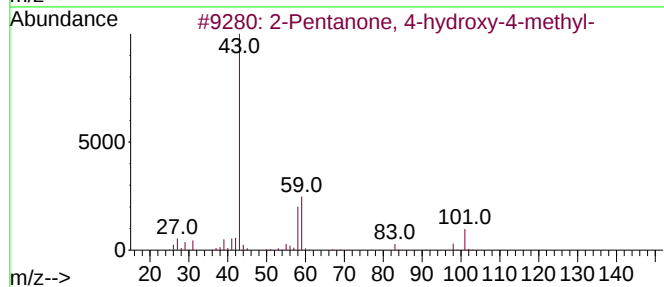
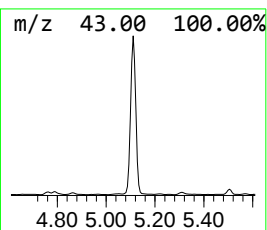
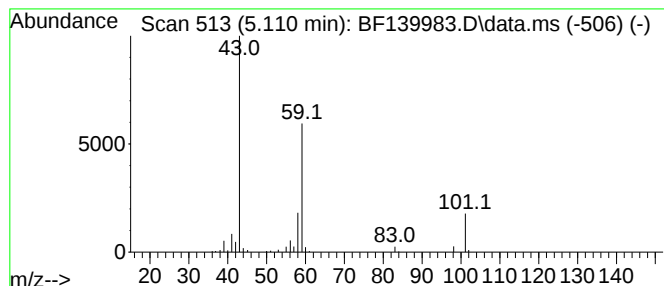
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.110	4.65 ng	174517	1,4-Dichlorobenzene-d4	6.893

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2			Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	42
3			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	37
4			3-Octanol	130	C8H18O	000589-98-0	36
5			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33



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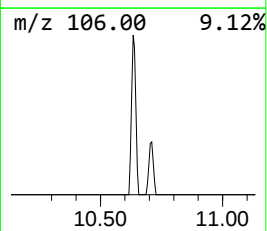
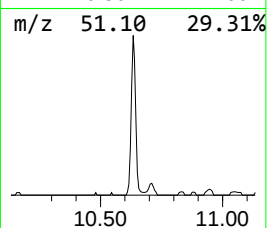
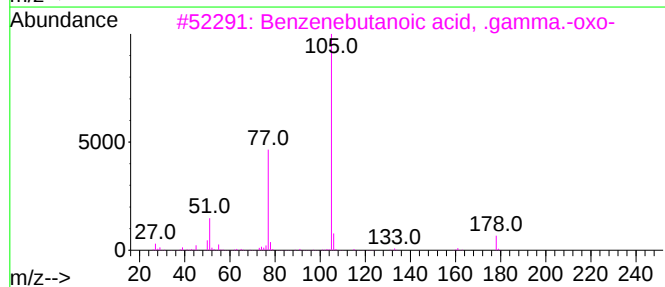
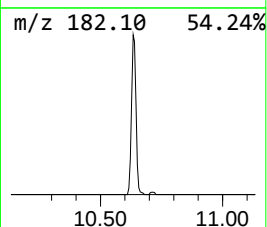
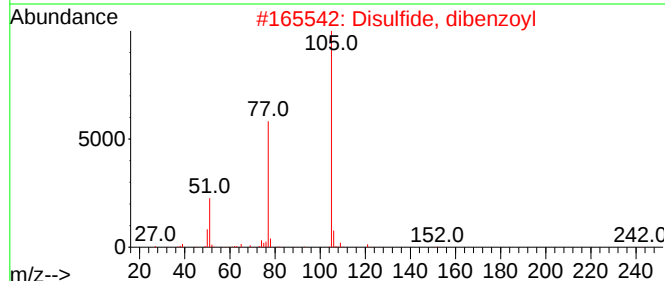
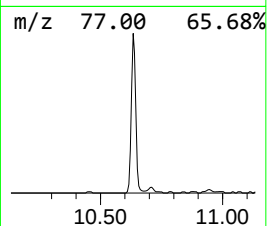
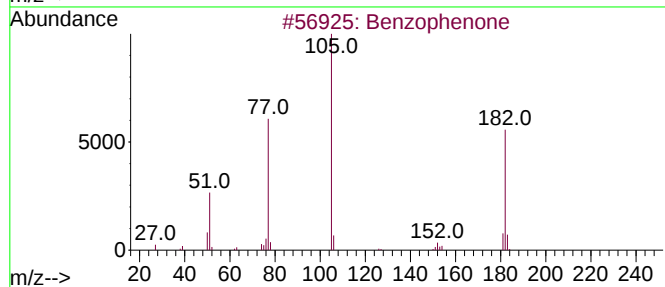
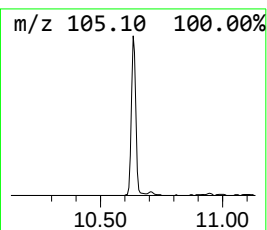
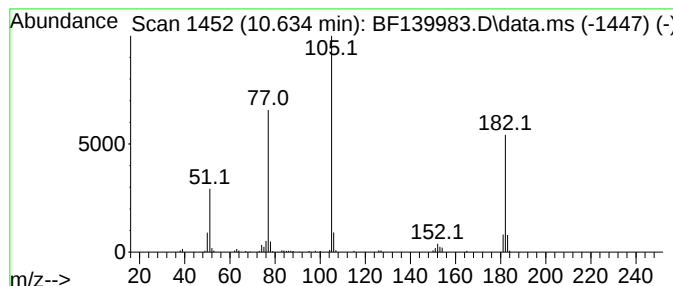
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Benzophenone Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.634	3.07 ng	133778	Acenaphthene-d10	9.922

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Disulfide, dibenzoyl	274	C14H10O2S2	000644-32-6	49
3			Benzenebutanoic acid, .gamma.-oxo-	178	C10H10O3	002051-95-8	47
4			Benzilamide	227	C14H13NO2	004746-87-6	47
5			N-Methoxy-N-methylbenzamide	165	C9H11NO2	006919-61-5	47



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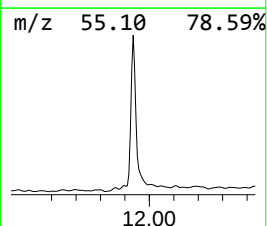
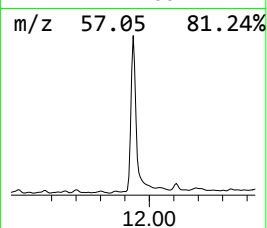
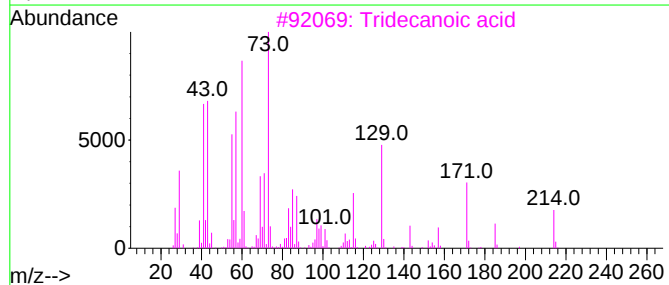
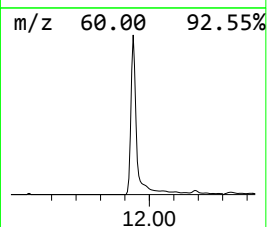
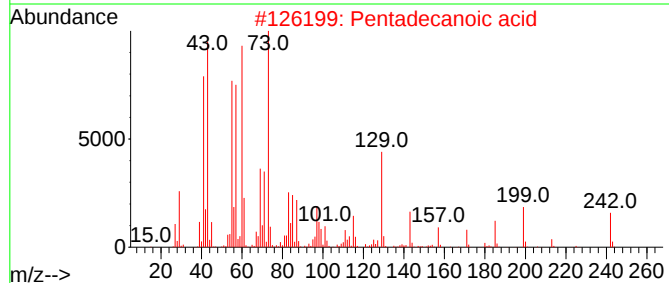
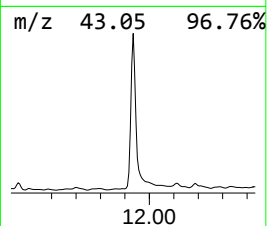
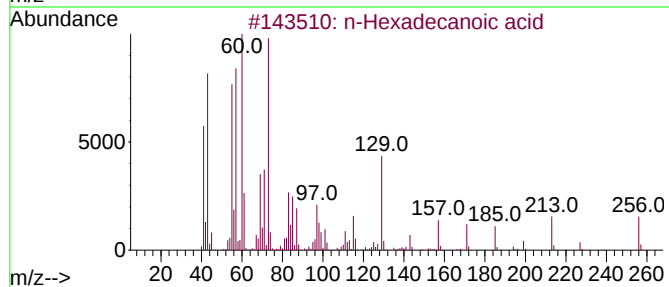
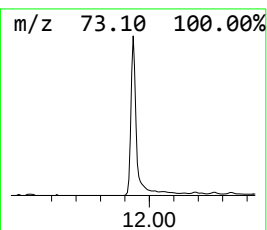
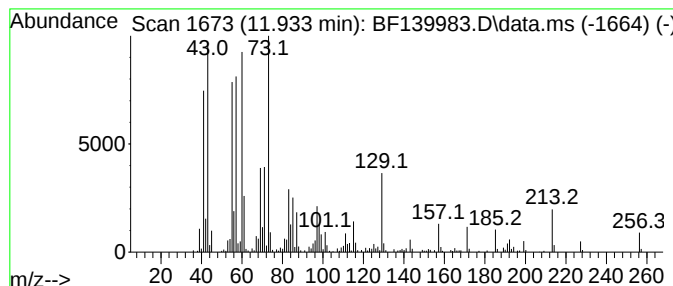
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.933	12.46 ng	511880	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	93
3			Tridecanoic acid	214	C13H26O2	000638-53-9	92
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5			8-Methylnonanoic acid	172	C10H20O2	005963-14-4	55



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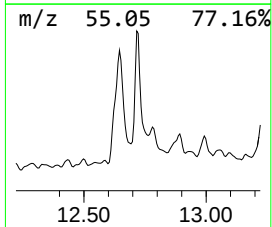
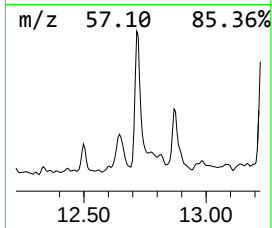
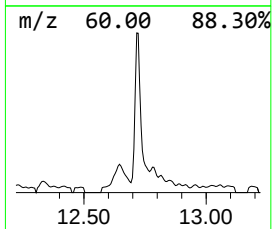
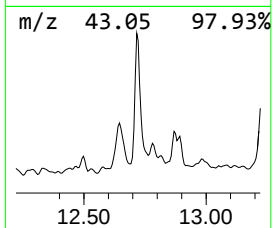
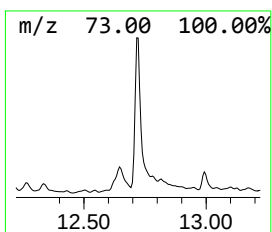
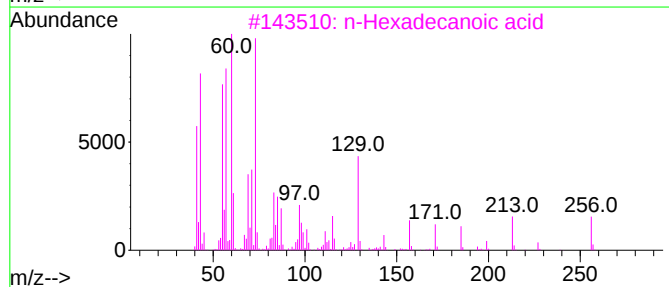
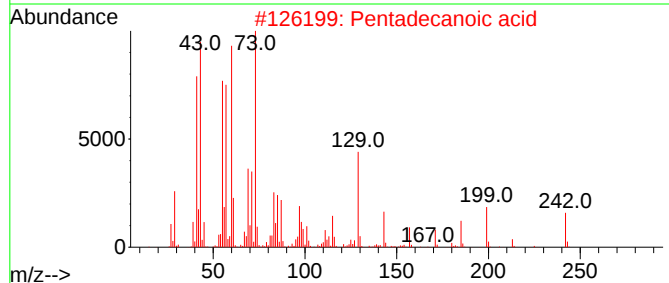
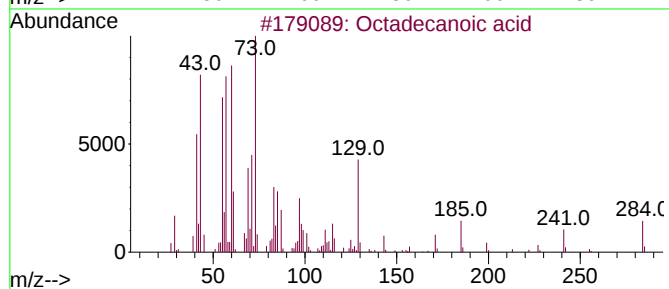
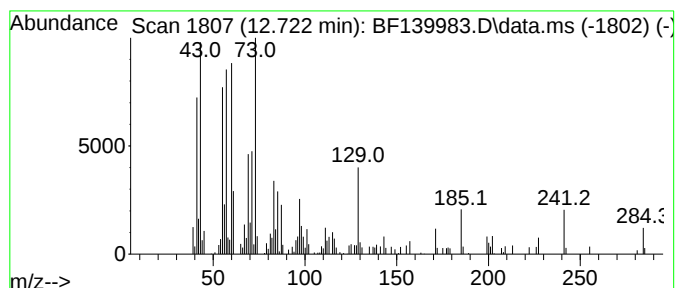
Instrument :
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Octadecanoic acid Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD		R.T.	
12.722	2.90 ng	119231	Phenanthrene-d10		11.410	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Octadecanoic acid		284	C18H36O2	000057-11-4	99
2	Pentadecanoic acid		242	C15H30O2	001002-84-2	91
3	n-Hexadecanoic acid		256	C16H32O2	000057-10-3	87
4	Octadecanoic acid, 2-(2-hydroxye...		372	C22H44O4	000106-11-6	86
5	Tetradecanoic acid		228	C14H28O2	000544-63-8	64



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Data File : BF139983.D
Acq On : 24 Oct 2024 00:11
Operator : RC/JU
Sample : P4385-14
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-7

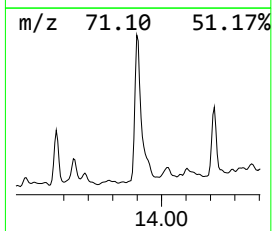
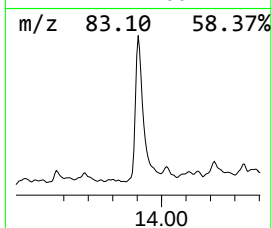
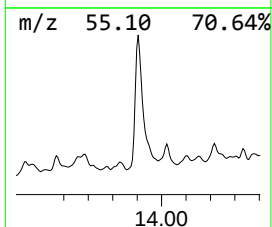
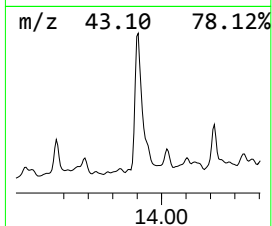
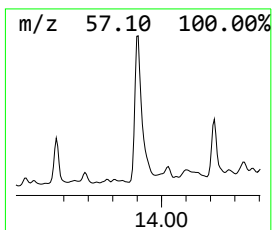
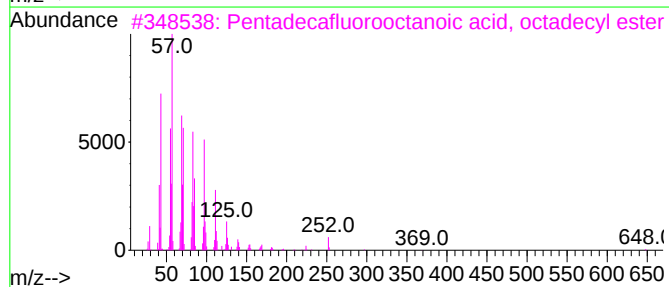
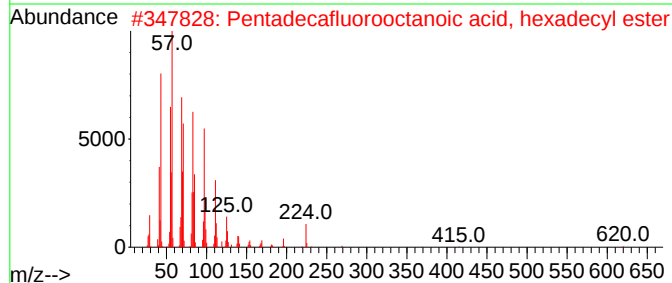
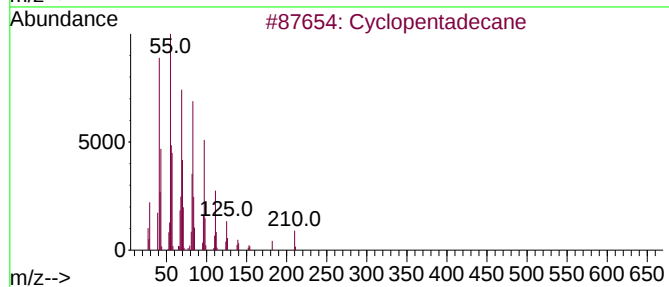
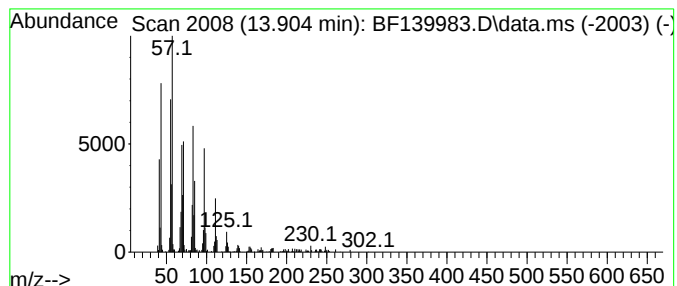
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Cyclopentadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.904	5.68 ng	291649	Chrysene-d12	14.051

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentadecane	210	C15H30	000295-48-7	95
2			Pentadecafluorooctanoic acid, he...	638	C24H33F15O2	1000406-04-6	94
3			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	94
4			Pentadecafluorooctanoic acid, pe...	624	C23H31F15O2	1000406-04-5	91
5			Tetracosyl heptafluorobutyrate	550	C28H49F7O2	1000351-83-7	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102324\
Data File : BF139983.D
Acq On : 24 Oct 2024 00:11
Operator : RC/JU
Sample : P4385-14
Misc :
ALS Vial : 20 Sample Multiplier: 1

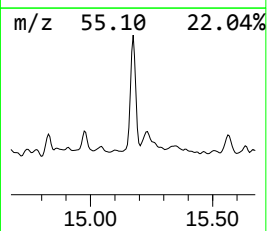
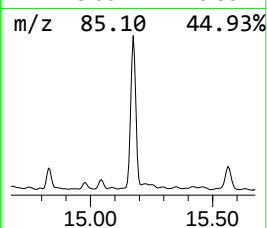
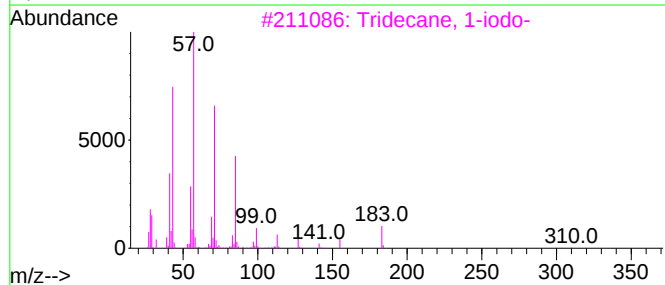
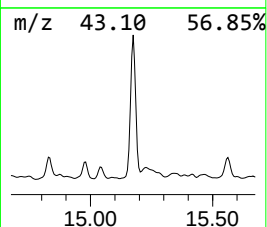
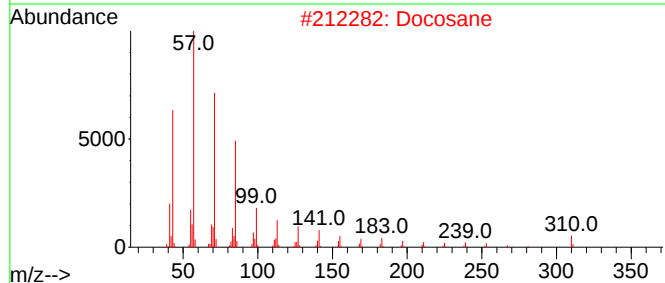
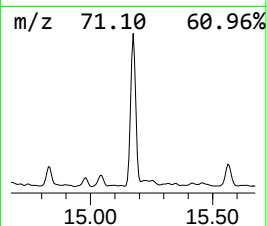
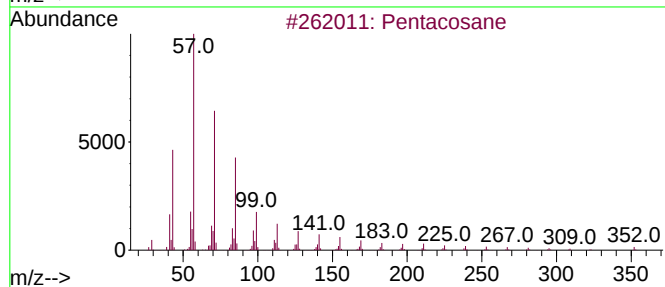
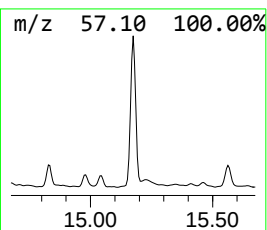
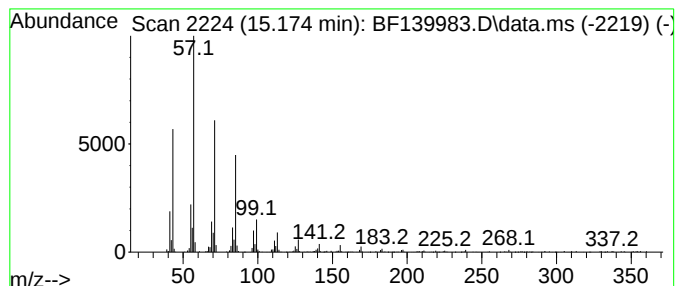
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Pentacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.174	9.36 ng	328069	Perylene-d12	15.527	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentacosane	352	C25H52	000629-99-2	97
2	Docosane	310	C22H46	000629-97-0	96
3	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	93
4	Octacosane	394	C28H58	000630-02-4	91
5	Hexacosane	366	C26H54	000630-01-3	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102324\
Data File : BF139983.D
Acq On : 24 Oct 2024 00:11
Operator : RC/JU
Sample : P4385-14
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-7

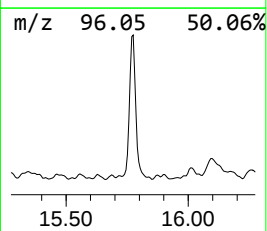
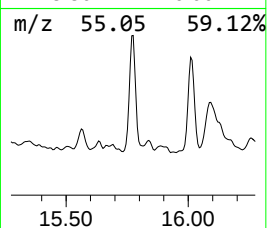
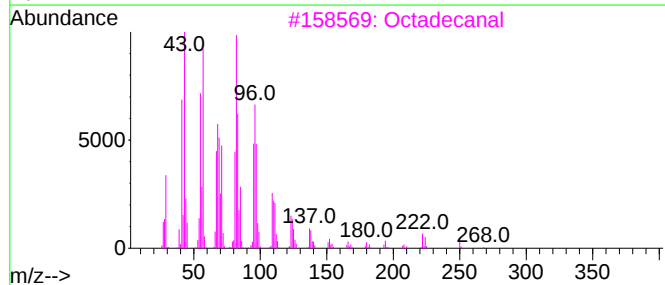
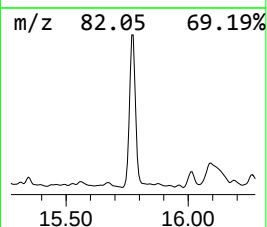
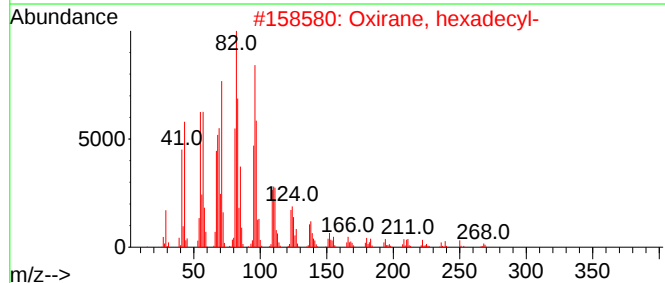
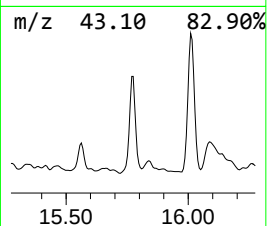
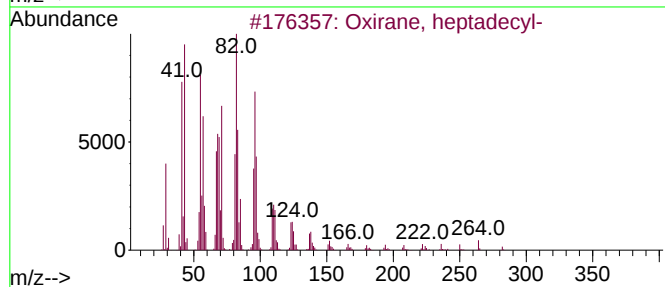
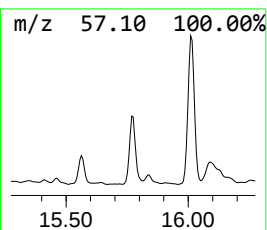
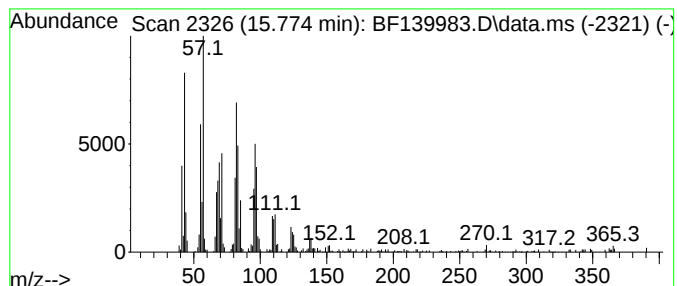
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Oxirane, heptadecyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.774	7.19 ng	251901	Perylene-d12	15.527

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Oxirane, heptadecyl-	282	C19H38O	067860-04-2	95
2			Oxirane, hexadecyl-	268	C18H36O	007390-81-0	91
3			Octadecanal	268	C18H36O	000638-66-4	90
4			Pentacosanal	366	C25H50O	058196-28-4	90
5			Octacosanal	408	C28H56O	022725-64-0	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102324\
Data File : BF139983.D
Acq On : 24 Oct 2024 00:11
Operator : RC/JU
Sample : P4385-14
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-7

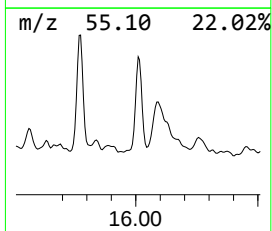
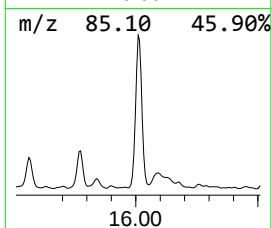
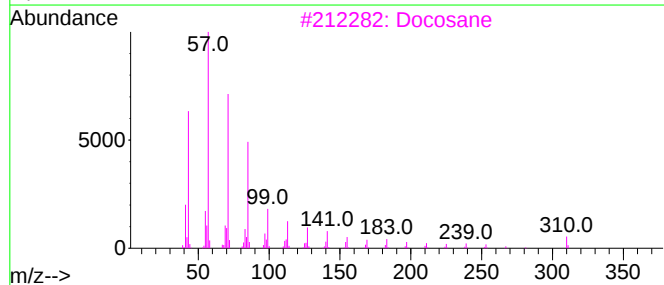
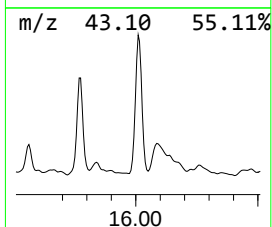
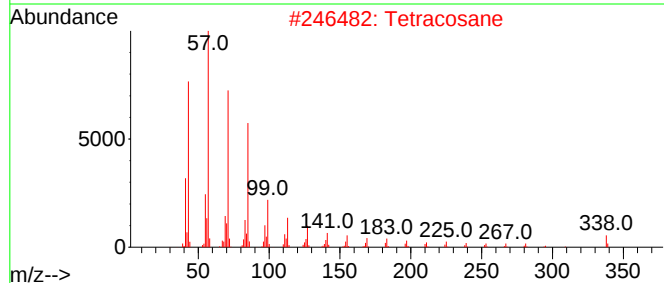
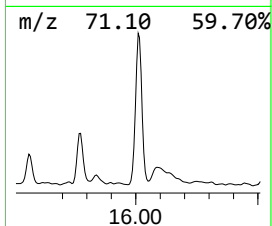
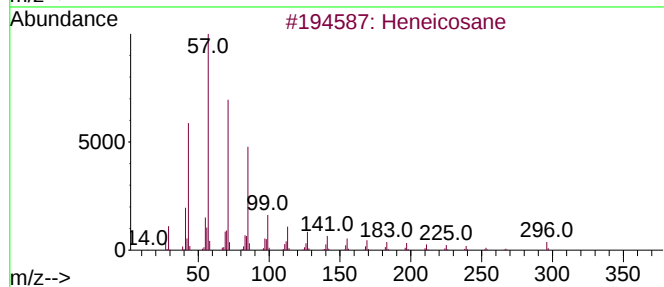
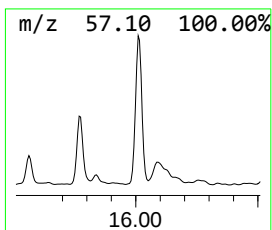
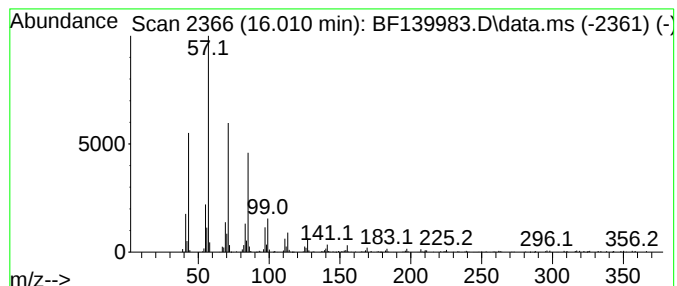
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Heneicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.010	8.14 ng	285153	Perylene-d12	15.527

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heneicosane	296	C21H44	000629-94-7	97
2			Tetracosane	338	C24H50	000646-31-1	96
3			Docosane	310	C22H46	000629-97-0	93
4			2-Bromo dodecane	248	C12H25Br	013187-99-0	93
5			Hexacosane	366	C26H54	000630-01-3	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102324\
Data File : BF139983.D
Acq On : 24 Oct 2024 00:11
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Sample : P4385-14
Misc :
ALS Vial : 20 Sample Multiplier: 1

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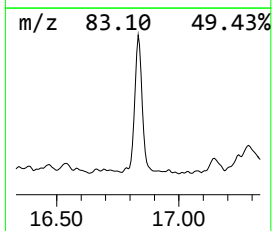
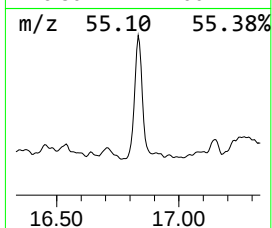
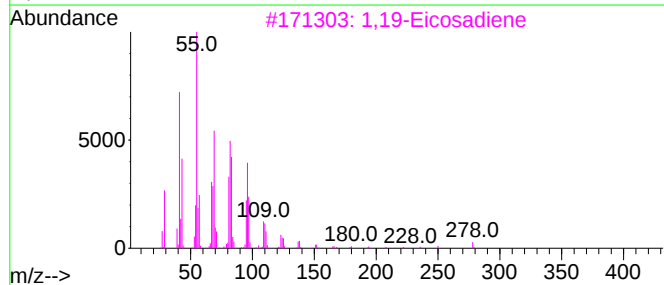
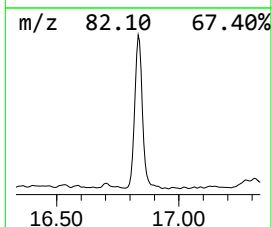
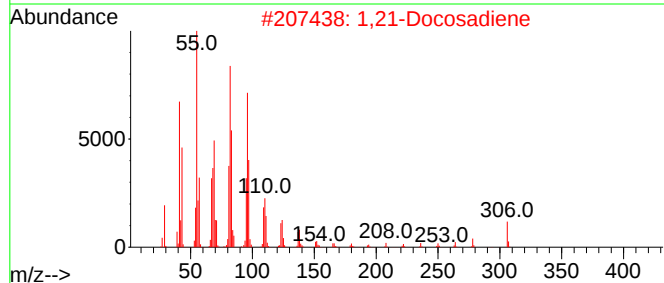
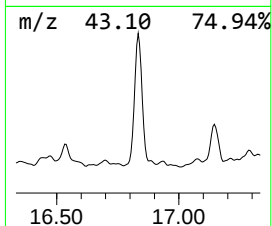
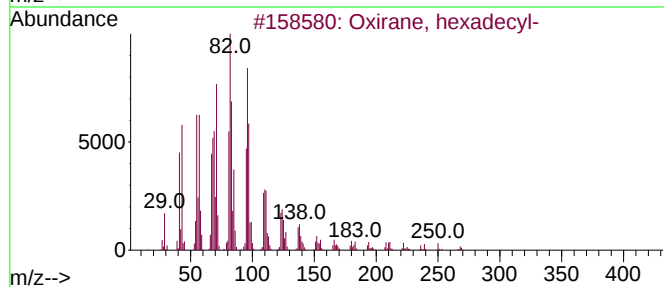
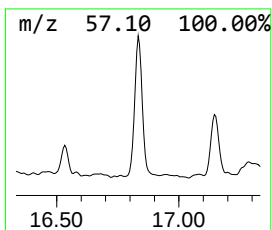
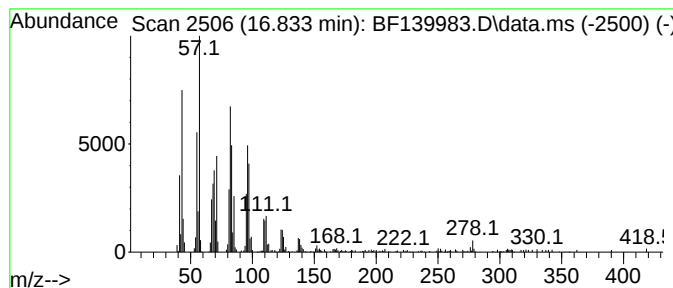
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Oxirane, hexadecyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.833	10.19 ng	356891	Perylene-d12	15.527

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Oxirane, hexadecyl-	268	C18H36O	007390-81-0	94
2			1,21-Docosadiene	306	C22H42	053057-53-7	93
3			1,19-Eicosadiene	278	C20H38	014811-95-1	93
4			E-8-Octadecacene-1-ol acetate	310	C20H38O2	002195-90-6	87
5			Docosanal	324	C22H44O	057402-36-5	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102324\
Data File : BF139983.D
Acq On : 24 Oct 2024 00:11
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Sample : P4385-14
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ALS Vial : 20 Sample Multiplier: 1

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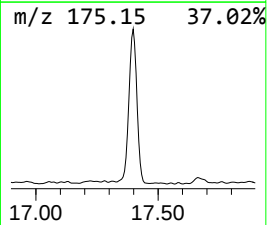
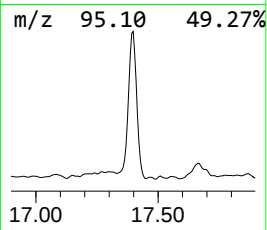
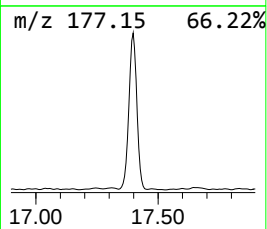
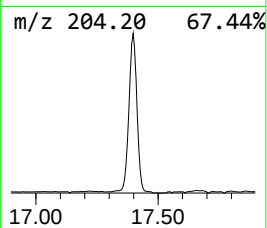
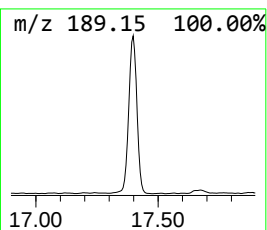
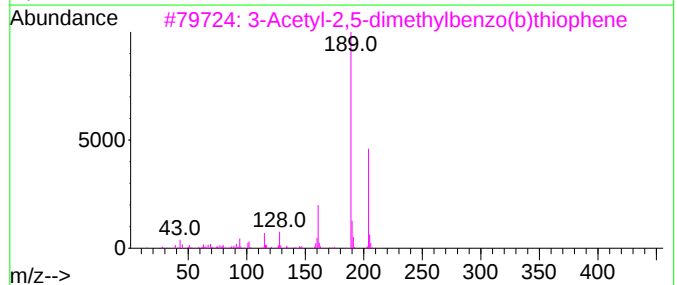
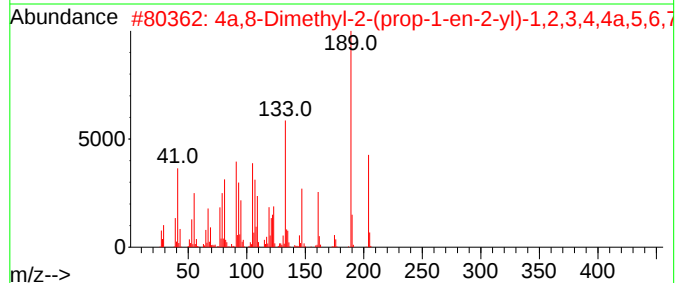
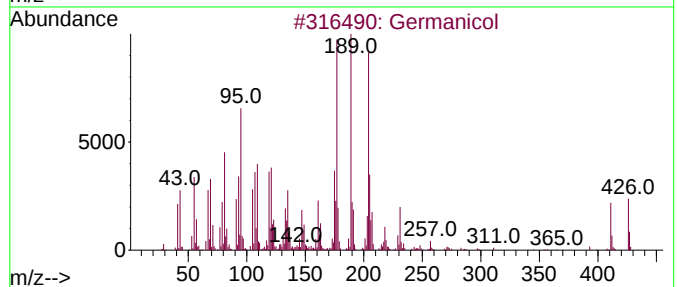
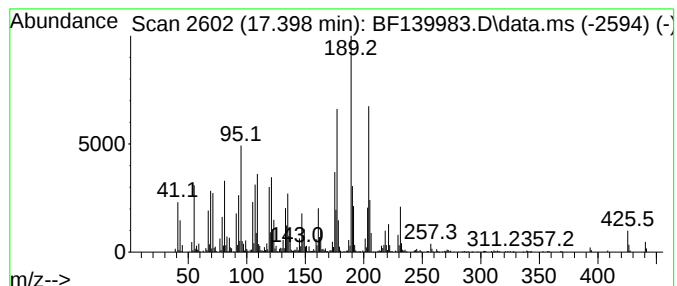
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Germanicol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.398	32.97 ng	1155060	Perylene-d12	15.527

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Germanicol	426	C30H50O	000465-02-1	58
2			4a,8-Dimethyl-2-(prop-1-en-2-yl)...	204	C15H24	103827-22-1	43
3			3-Acetyl-2,5-dimethylbenzo(b)thi...	204	C12H12OS	006179-04-0	38
4			Naphthalene, decahydro-4a-methyl...	204	C15H24	000515-17-3	35
5			2-Acetyl-1-methyl-3-indolyl acetate	231	C13H13NO3	061153-69-3	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102324\
Data File : BF139983.D
Acq On : 24 Oct 2024 00:11
Operator : RC/JU
Sample : P4385-14
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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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\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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2-Pentanone, 4-...	5.110	4.7	ng	174517	1	6.893	750253	20.0
Benzophenone	10.634	3.1	ng	133778	3	9.922	870790	20.0
n-Hexadecanoic ...	11.933	12.5	ng	511880	4	11.410	821629	20.0
Octadecanoic acid	12.722	2.9	ng	119231	4	11.410	821629	20.0
Cyclopentadecane	13.904	5.7	ng	291649	5	14.051	1027510	20.0
Pentacosane	15.174	9.4	ng	328069	6	15.527	700705	20.0
Oxirane, heptad...	15.774	7.2	ng	251901	6	15.527	700705	20.0
Heneicosane	16.010	8.1	ng	285153	6	15.527	700705	20.0
Oxirane, hexade...	16.833	10.2	ng	356891	6	15.527	700705	20.0
Germanicol	17.398	33.0	ng	1155060	6	15.527	700705	20.0