

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF031124\
 Data File : BF137566.D
 Acq On : 11 Mar 2024 20:18
 Operator : CG\JU
 Sample : P1701-01
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 RCA-1-COMP

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-BF022924.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF137566.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.263	23	30	41	rVB	1323459	1851274	39.56%	4.612%
2	5.569	588	592	618	rBV	4456800	4398672	94.00%	10.958%
3	6.545	753	758	761	rBV	4378035	4232695	90.45%	10.544%
4	6.904	815	819	834	rBV	1376691	1351231	28.87%	3.366%
5	7.457	909	913	925	rBV	2732569	2825918	60.39%	7.040%
6	8.175	1029	1035	1041	rBV	1747395	1757878	37.56%	4.379%
7	8.769	1132	1136	1138	rBV	60406	59551	1.27%	0.148%
8	9.198	1206	1209	1213	rBV2	76547	73472	1.57%	0.183%
9	9.251	1214	1218	1221	rBV	5318968	4679611	100.00%	11.658%
10	9.333	1228	1232	1236	rVB	149641	134623	2.88%	0.335%
11	9.657	1284	1287	1289	rVB	75895	61151	1.31%	0.152%
12	9.792	1307	1310	1315	rBV5	39575	53867	1.15%	0.134%
13	9.869	1320	1323	1326	rBV	161418	130239	2.78%	0.324%
14	9.927	1327	1333	1337	rBV	2137857	1839583	39.31%	4.583%
15	10.033	1347	1351	1356	rVB2	102291	133713	2.86%	0.333%
16	10.251	1385	1388	1392	rBV2	60534	75631	1.62%	0.188%
17	10.369	1405	1408	1411	rVB	183656	148261	3.17%	0.369%
18	10.592	1444	1446	1450	rVB	124857	103257	2.21%	0.257%
19	10.645	1452	1455	1458	rVB3	48651	65855	1.41%	0.164%
20	10.721	1464	1468	1473	rBV	2218197	2064510	44.12%	5.143%
21	10.851	1486	1490	1497	rVB2	232955	370901	7.93%	0.924%
22	11.298	1564	1566	1568	rBV	137316	104112	2.22%	0.259%
23	11.327	1568	1571	1579	rVB	141840	159601	3.41%	0.398%
24	11.427	1584	1588	1590	rBV	1424020	1371092	29.30%	3.416%
25	11.451	1590	1592	1597	rVV	427848	364676	7.79%	0.908%
26	11.504	1598	1601	1605	rVB	97230	84762	1.81%	0.211%
27	11.668	1626	1629	1636	rBV4	132166	202894	4.34%	0.505%
28	11.727	1636	1639	1642	rVB	117351	96989	2.07%	0.242%
29	11.933	1671	1674	1676	rBV	79639	66477	1.42%	0.166%
30	11.974	1676	1681	1685	rVV2	165997	242389	5.18%	0.604%
31	12.045	1690	1693	1696	rBV	118142	112965	2.41%	0.281%
32	12.139	1707	1709	1712	rBV	78187	65106	1.39%	0.162%
33	12.221	1720	1723	1727	rBV2	192973	196592	4.20%	0.490%
34	12.486	1765	1768	1771	rBV	74650	81562	1.74%	0.203%
35	12.527	1771	1775	1780	rVV4	112801	198588	4.24%	0.495%
36	12.574	1780	1783	1786	rVV3	51401	57142	1.22%	0.142%

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37	12.645	1792	1795	1801	rBV	835499	821158	17.55%	2.046%
38	12.880	1829	1835	1838	rBV	797256	893952	19.10%	2.227%
39	12.910	1838	1840	1842	rVV2	80120	73724	1.58%	0.184%
40	12.939	1842	1845	1848	rVB2	50966	60004	1.28%	0.149%
41	13.027	1857	1860	1868	rVB	3612249	3388744	72.42%	8.442%
42	13.210	1889	1891	1895	rVB	125287	120288	2.57%	0.300%
43	13.274	1899	1902	1906	rVB2	93093	106120	2.27%	0.264%
44	13.315	1906	1909	1912	rBV	103559	99210	2.12%	0.247%
45	13.951	2013	2017	2025	rBV3	213353	304346	6.50%	0.758%
46	14.092	2036	2041	2043	rBV2	1347675	1647547	35.21%	4.104%
47	14.115	2043	2045	2052	rVB	421561	398640	8.52%	0.993%
48	14.198	2057	2059	2061	rVB	71960	55837	1.19%	0.139%
49	14.998	2192	2195	2200	rVB2	111749	129499	2.77%	0.323%
50	15.180	2222	2226	2230	rBV	302134	504327	10.78%	1.256%
51	15.292	2243	2245	2250	rVB2	111858	123676	2.64%	0.308%
52	15.509	2278	2282	2289	rVB	165845	258406	5.52%	0.644%
53	15.574	2289	2293	2300	rBV	225339	357204	7.63%	0.890%
54	15.645	2300	2305	2310	rBV	702828	982748	21.00%	2.448%

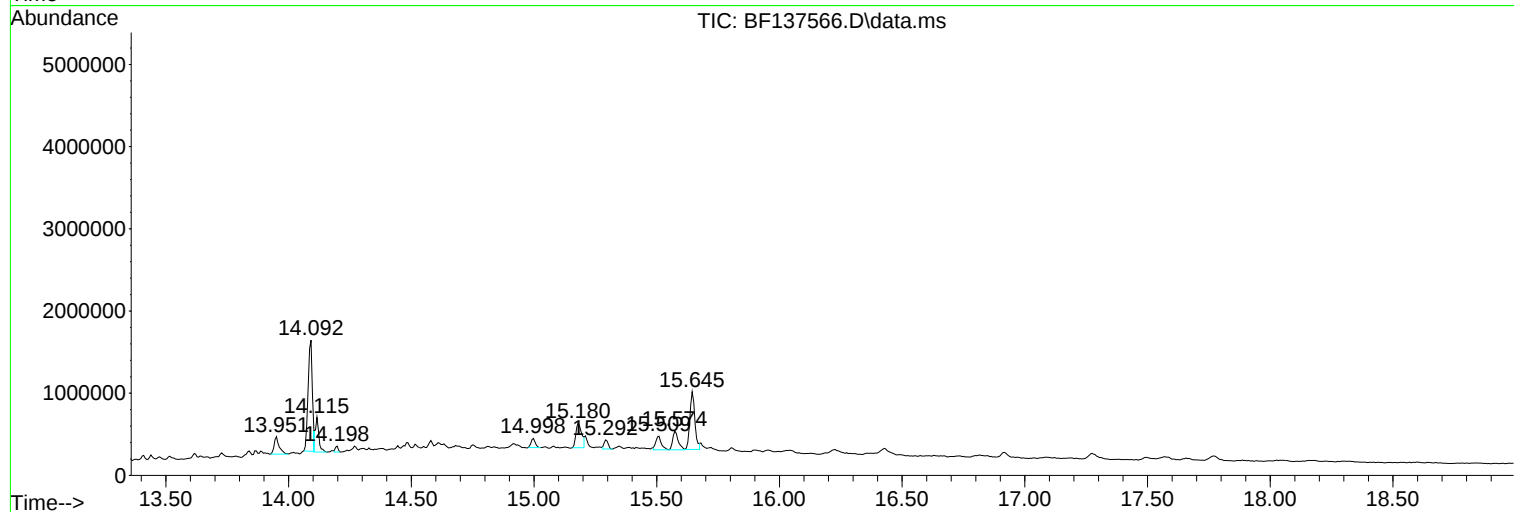
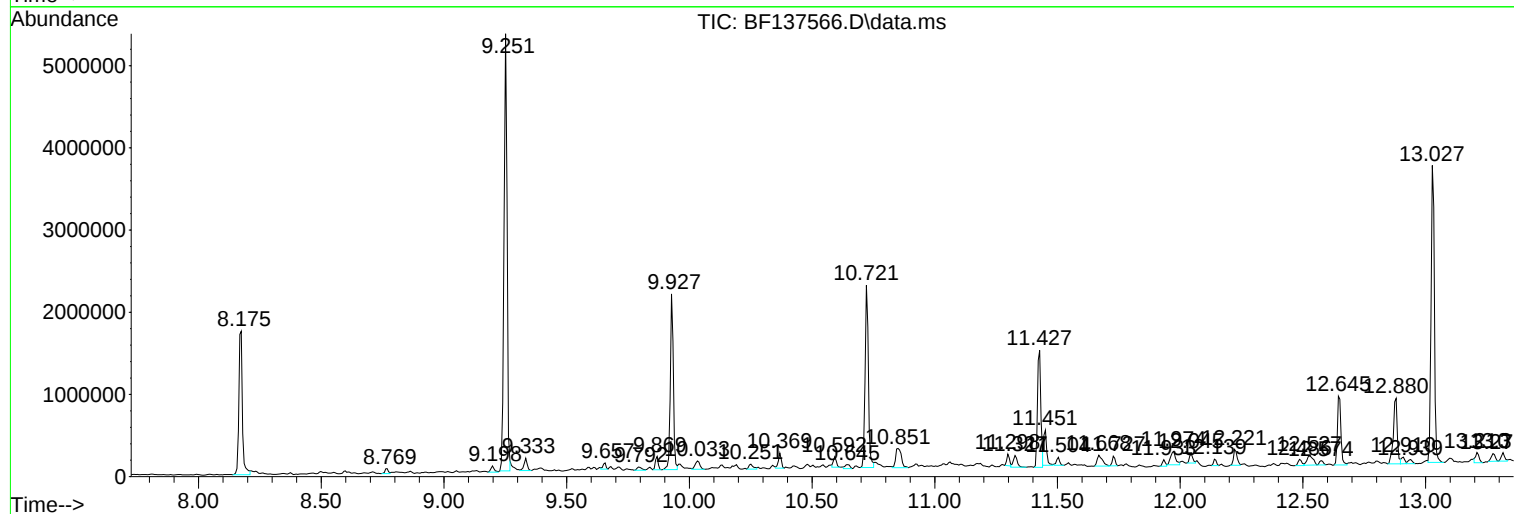
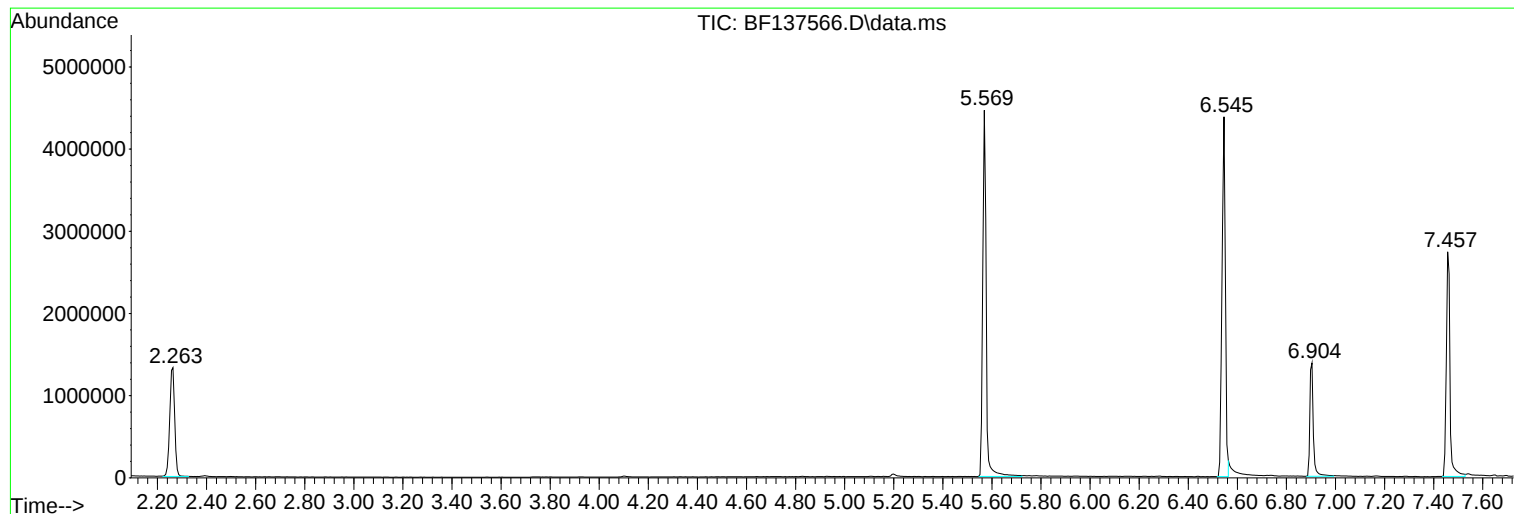
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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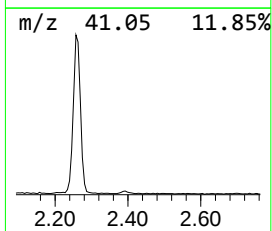
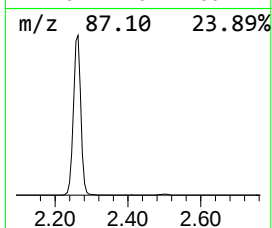
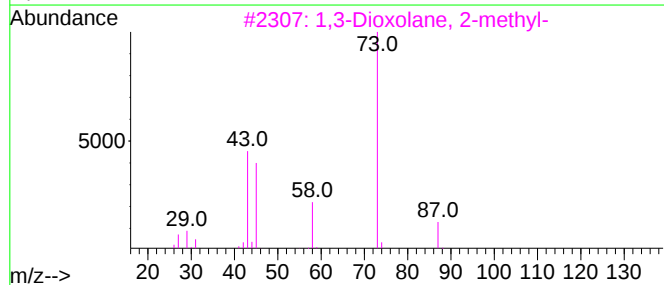
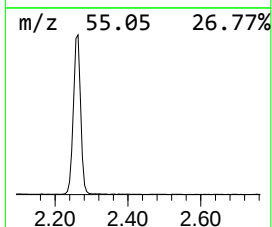
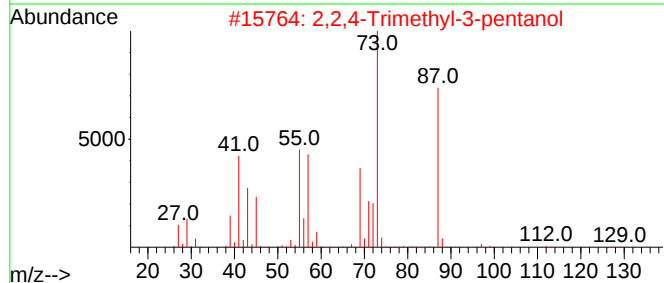
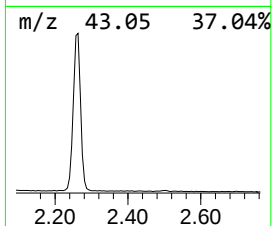
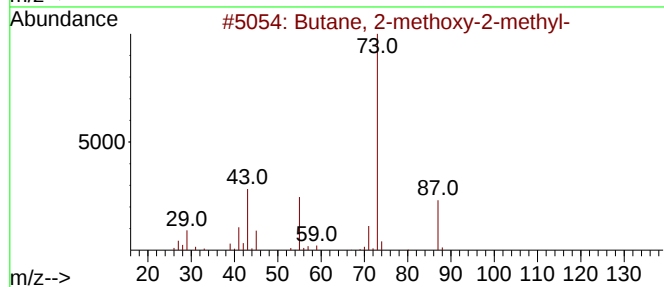
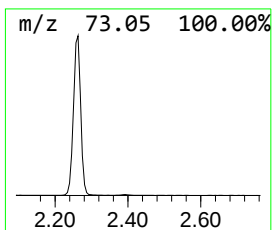
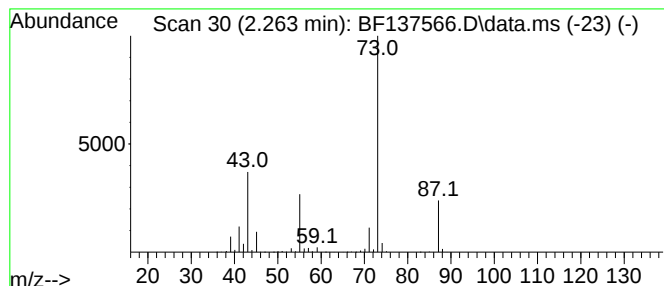
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.263	27.40 ng	1851270	1,4-Dichlorobenzene-d4	6.904

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	37
4			3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	37
5			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17



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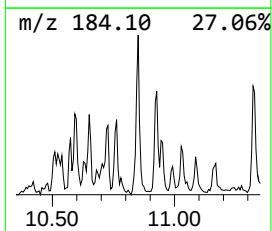
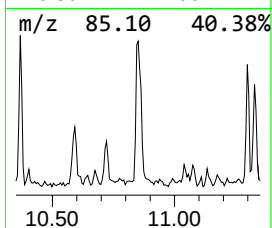
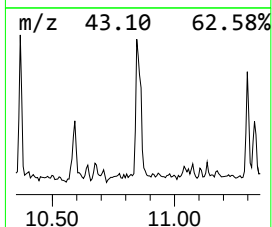
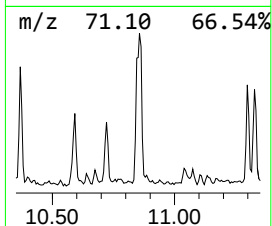
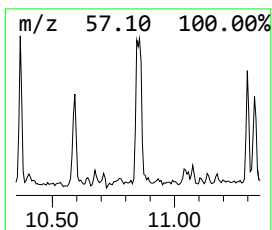
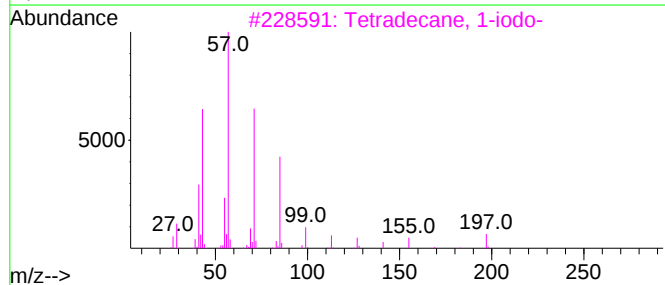
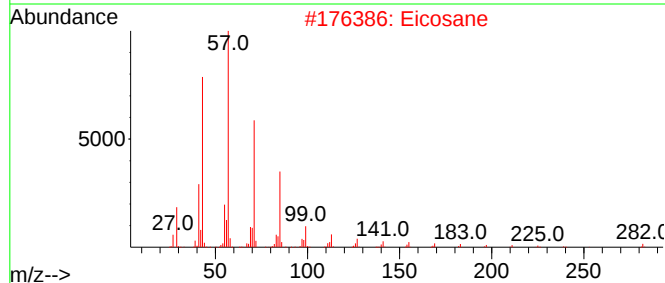
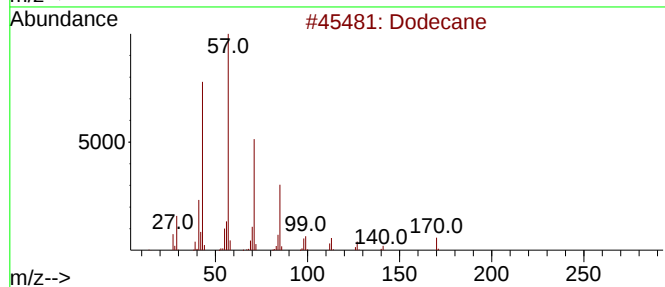
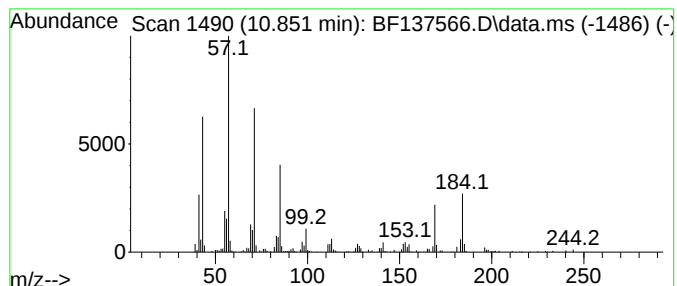
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Dodecane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.851	5.41 ng	370901	Phenanthrene-d10	11.427

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecane	170	C12H26	000112-40-3	64
2			Eicosane	282	C20H42	000112-95-8	62
3			Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	62
4			Heptacosane	380	C27H56	000593-49-7	62
5			Octacosane	394	C28H58	000630-02-4	62



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ALS Vial : 15 Sample Multiplier: 1

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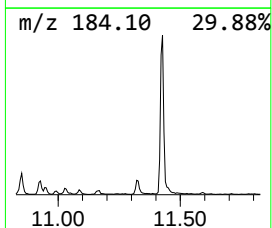
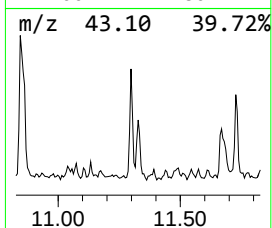
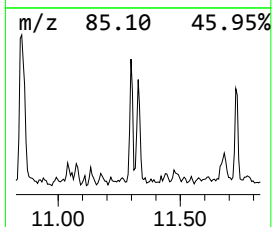
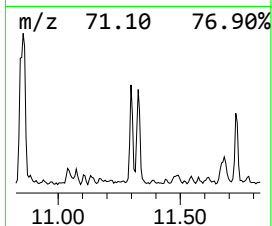
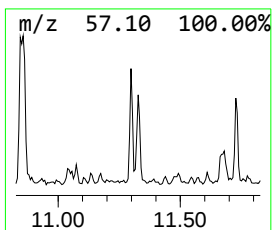
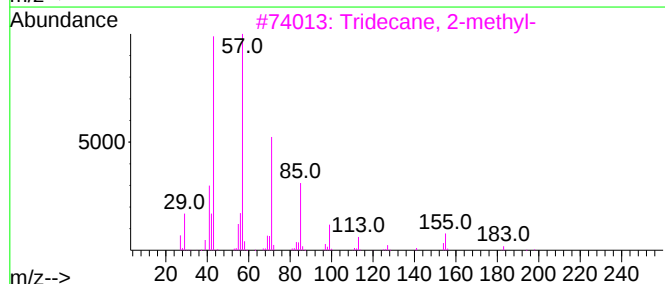
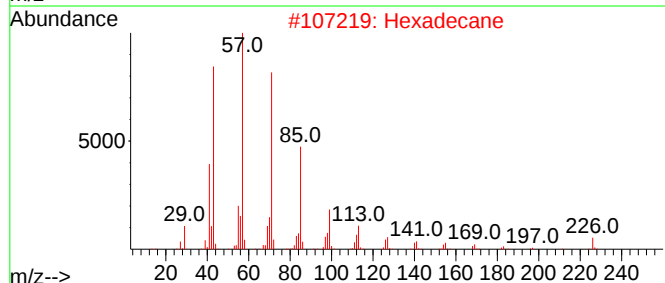
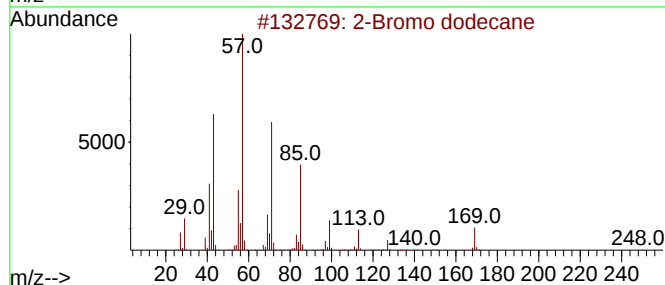
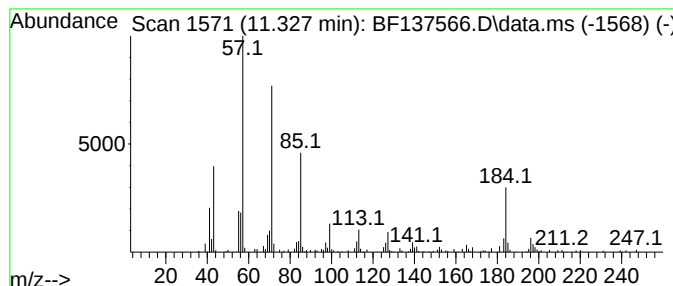
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 2-Bromo dodecane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.327	2.33 ng	159601	Phenanthrene-d10	11.427

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Bromo dodecane	248	C12H25Br	013187-99-0	80
2		Hexadecane	226	C16H34	000544-76-3	74
3		Tridecane, 2-methyl-	198	C14H30	001560-96-9	64
4		Sulfurous acid, butyl nonyl ester	264	C13H28O3S	1000309-17-6	59
5		Dodecane, 2,7,10-trimethyl-	212	C15H32	074645-98-0	58



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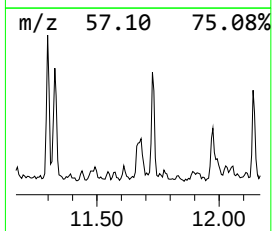
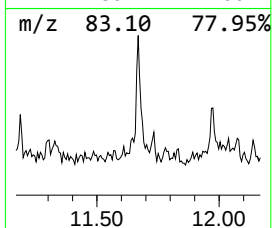
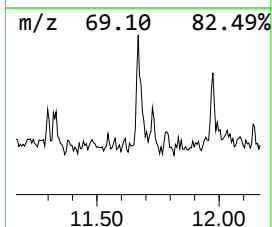
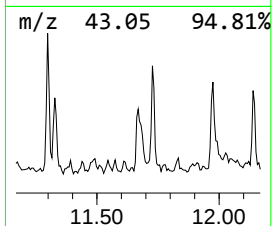
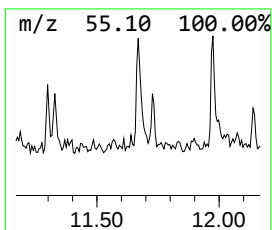
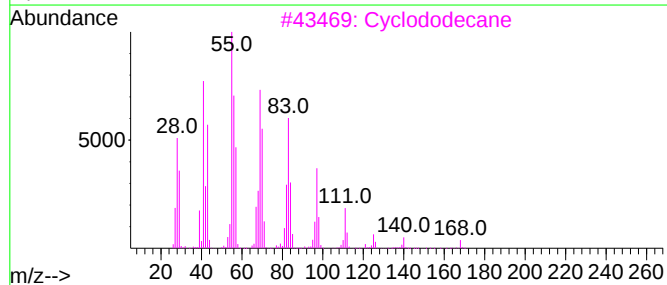
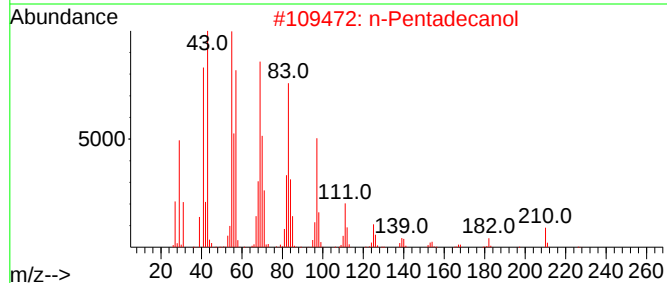
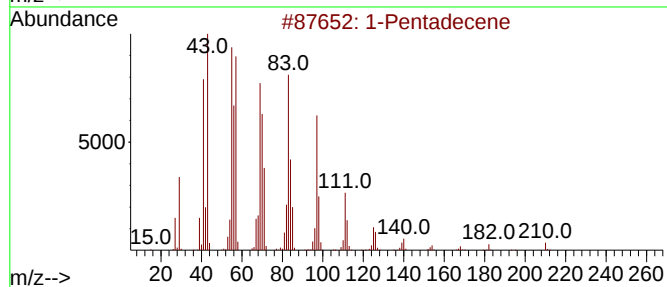
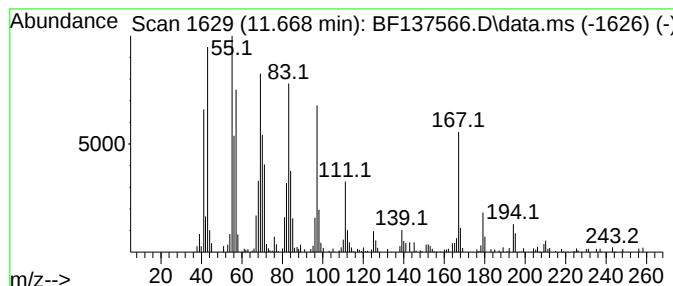
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 1-Pentadecene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.669	2.96 ng	202894	Phenanthrene-d10	11.427

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Pentadecene	210	C15H30	013360-61-7	99
2			n-Pentadecanol	228	C15H32O	000629-76-5	95
3			Cyclododecane	168	C12H24	000294-62-2	93
4			9-Octadecene, (E)-	252	C18H36	007206-25-9	87
5			1-Nonadecene	266	C19H38	018435-45-5	87



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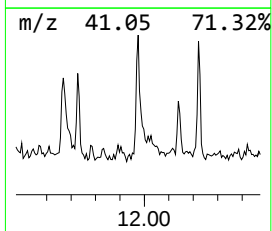
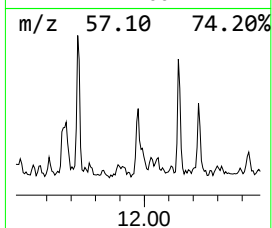
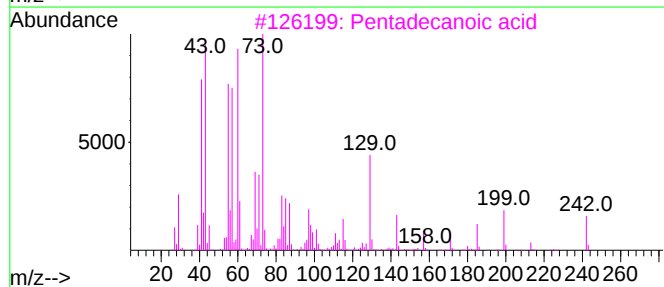
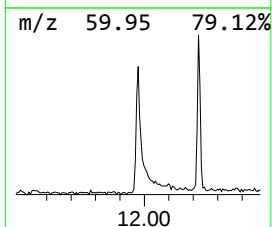
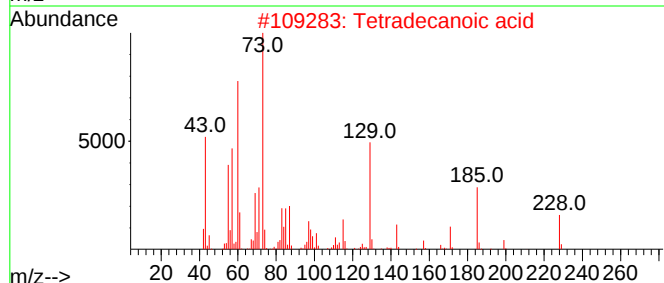
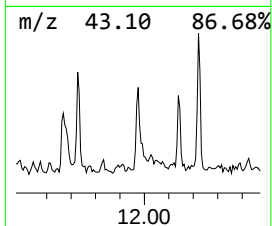
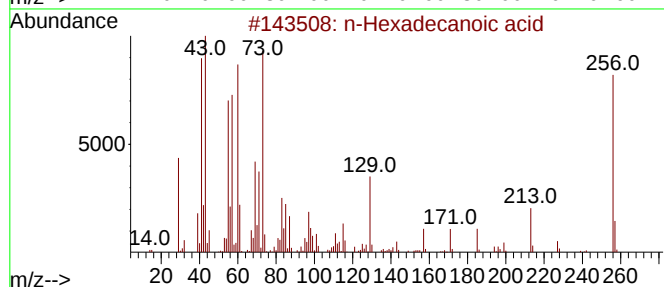
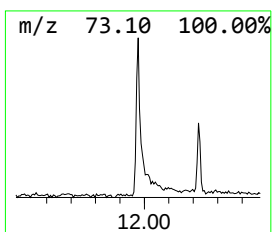
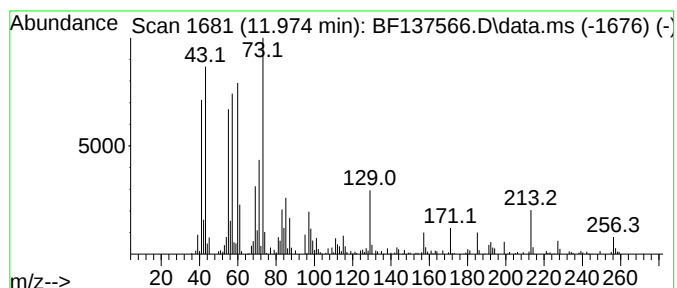
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ClientSampleId :
RCA-1-COMP

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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 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.974	3.54 ng	242389	Phenanthrene-d10	11.427	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	89
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	76
4	Tridecanoic acid	214	C13H26O2	000638-53-9	70
5	Tetradecane, 2,6,10-trimethyl-	240	C17H36	014905-56-7	44



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF031124\
Data File : BF137566.D
Acq On : 11 Mar 2024 20:18
Operator : CG\JU
Sample : P1701-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RCA-1-COMP

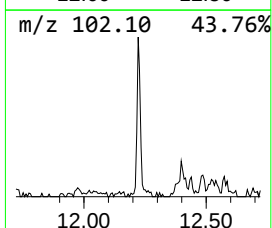
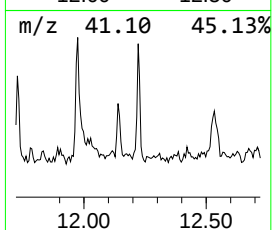
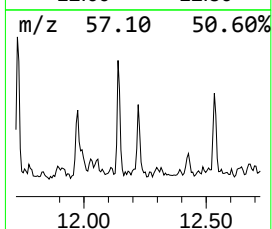
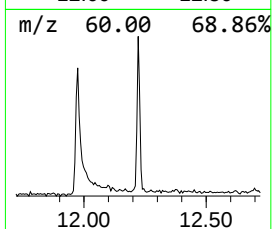
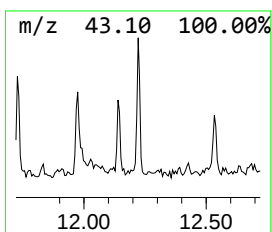
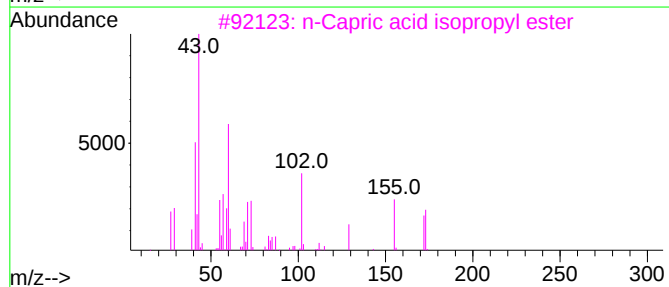
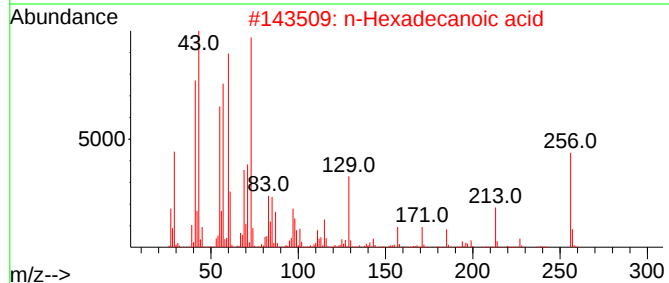
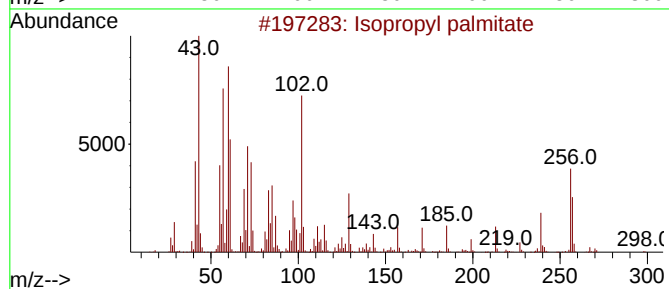
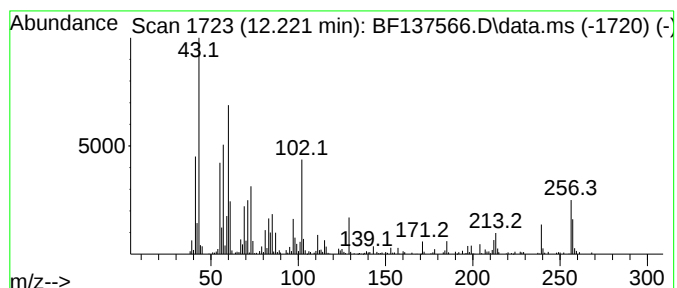
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Isopropyl palmitate Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.221	2.87 ng	196592	Phenanthrene-d10	11.427

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Isopropyl palmitate	298	C19H38O2	000142-91-6	87
2		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	64
3		n-Capric acid isopropyl ester	214	C13H26O2	002311-59-3	50
4		Heptanoic acid, 2,2-dimethyl-6-o...	186	C10H18O3	000926-27-2	30
5		Acetamide, N,N'-carbonylbis-	144	C5H8N2O3	000638-20-0	22



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF031124\
Data File : BF137566.D
Acq On : 11 Mar 2024 20:18
Operator : CG\JU
Sample : P1701-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

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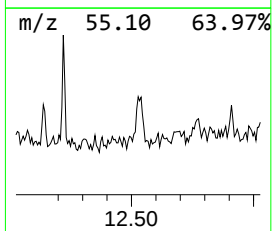
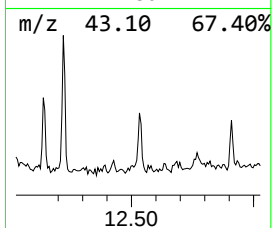
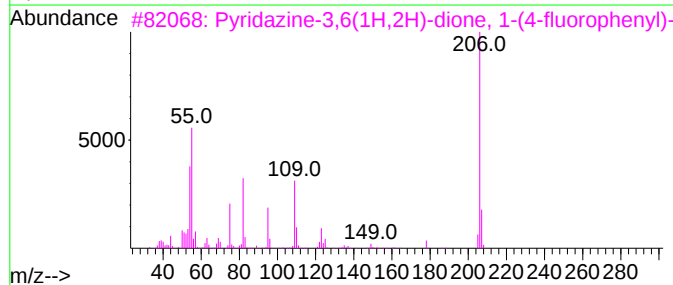
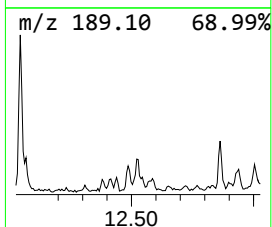
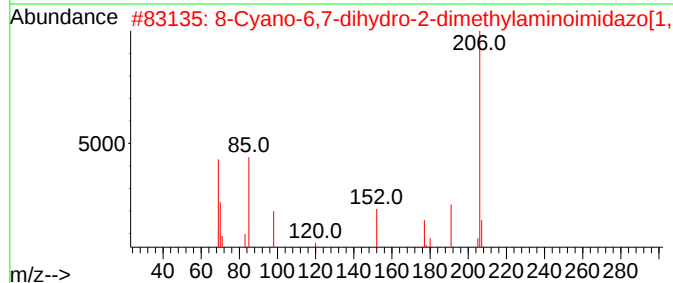
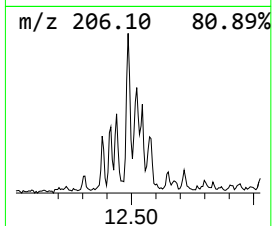
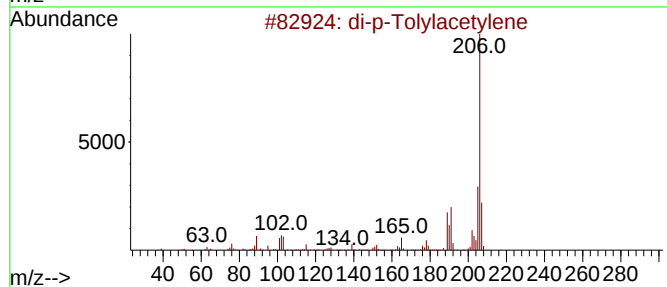
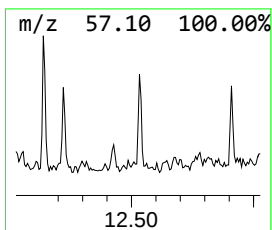
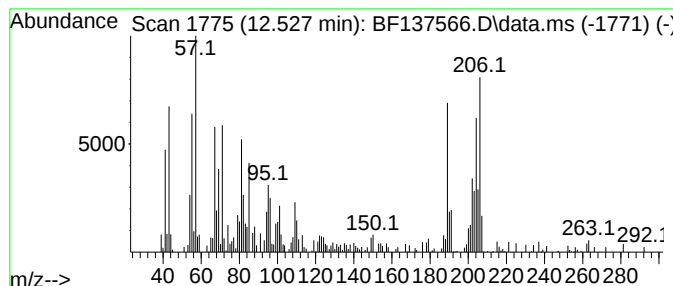
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown12.527 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.527	2.90 ng	198588	Phenanthrene-d10	11.427

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			di-p-Tolylacetylene	206	C16H14	002789-88-0	38
2			8-Cyano-6,7-dihydro-2-dimethylam...	206	C8H10N6O	077455-10-8	38
3			Pyridazine-3,6(1H,2H)-dione, 1-(...	206	C10H7FN2O2	075222-34-3	35
4			1,3-Butadiene, 1,4-diphenyl-, (E...	206	C16H14	000538-81-8	30
5			7-Methoxy-6-methyl-2,4-pteridine...	206	C8H10N6O	343347-40-0	30



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF031124\
Data File : BF137566.D
Acq On : 11 Mar 2024 20:18
Operator : CG\JU
Sample : P1701-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

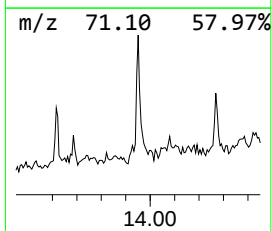
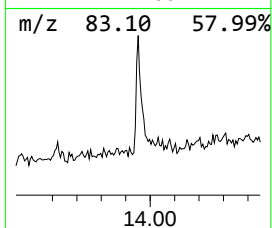
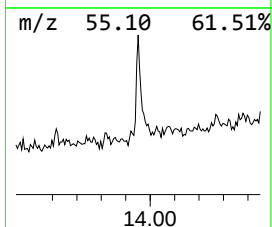
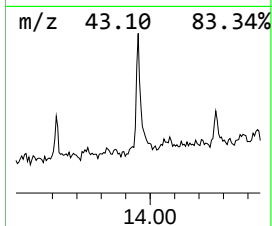
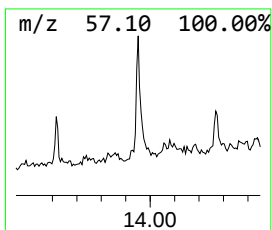
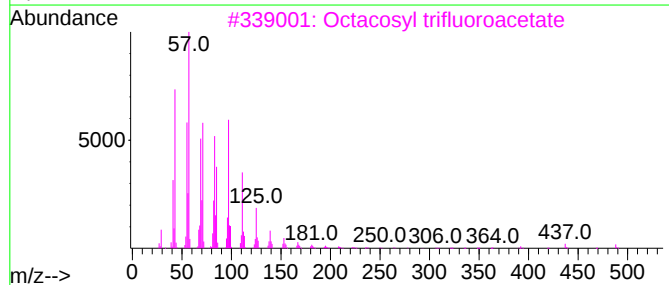
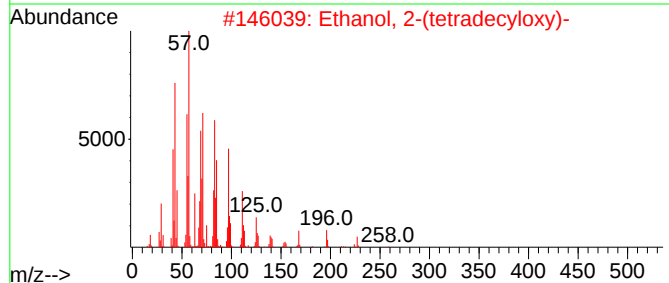
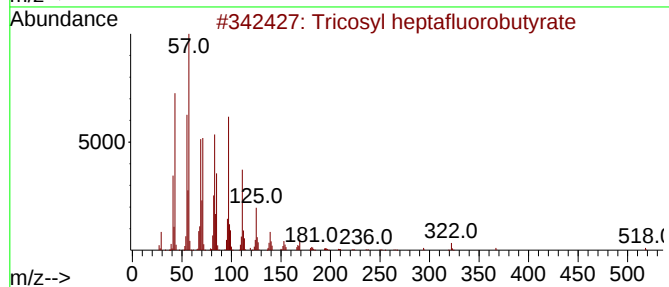
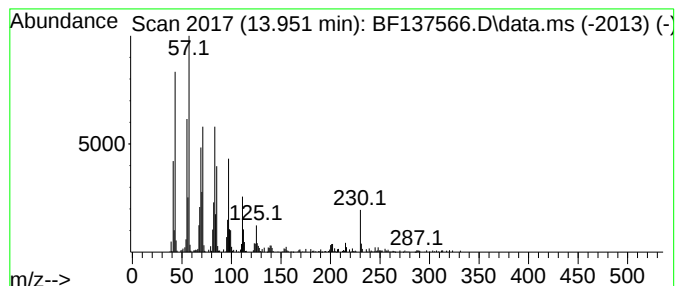
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Tricosyl heptafluorobutyrate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.951	3.69 ng	304346	Chrysene-d12	14.092	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tricosyl heptafluorobutyrate	536	C27H47F7O2	1000351-83-4	90
2	Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	90
3	Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	90
4	Tetracosyl heptafluorobutyrate	550	C28H49F7O2	1000351-83-7	87
5	Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	81



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF031124\
Data File : BF137566.D
Acq On : 11 Mar 2024 20:18
Operator : CG\JU
Sample : P1701-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

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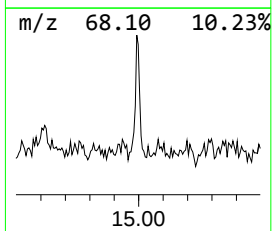
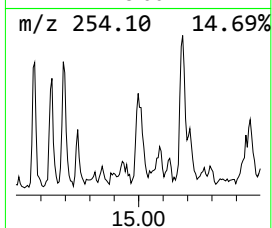
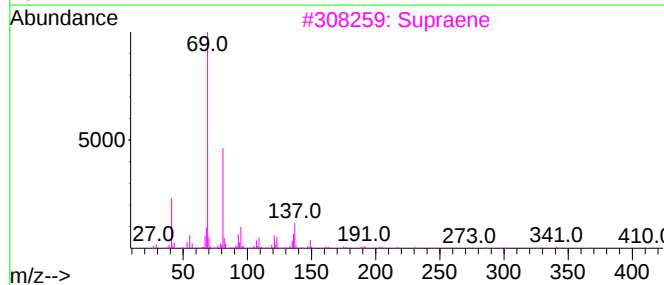
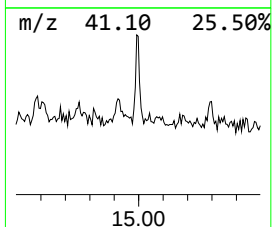
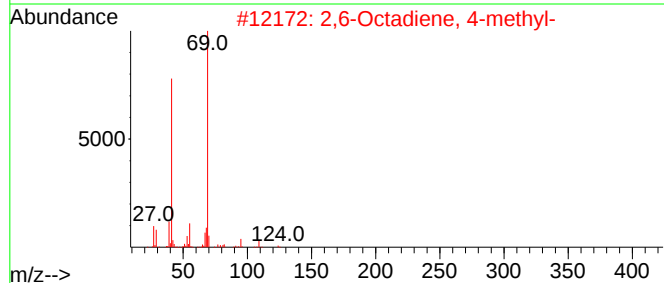
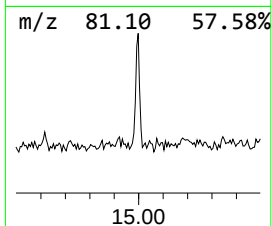
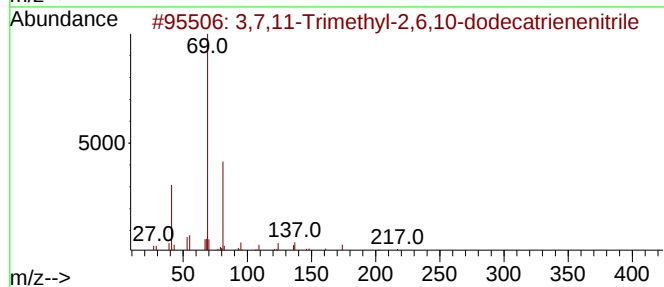
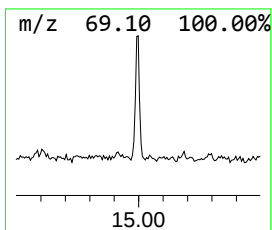
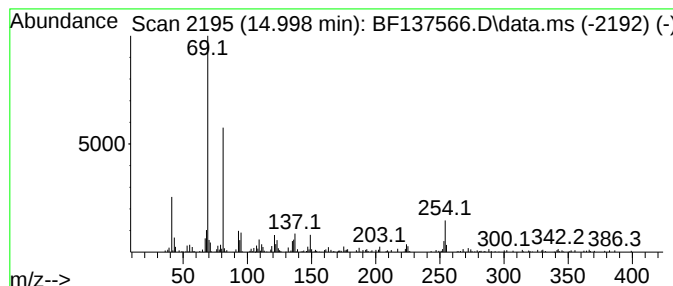
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 3,7,11-Trimethyl-2,6,10-dod... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.998	2.64 ng	129499	Perylene-d12	15.645

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	3,7,11-Trimethyl-2,6,10-dodecatr...	217	C15H23N	029789-67-1	64		
2	2,6-Octadiene, 4-methyl-	124	C9H16	074498-94-5	59		
3	Supraene	410	C30H50	007683-64-9	59		
4	1,3-Dioxolan-2-one, 3-methyl-3-(...	264	C16H24O3	336879-76-6	59		
5	(E)-2-Butenoic acid, 2-(methylen...	180	C11H16O2	1000158-24-3	59		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF031124\
Data File : BF137566.D
Acq On : 11 Mar 2024 20:18
Operator : CG\JU
Sample : P1701-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

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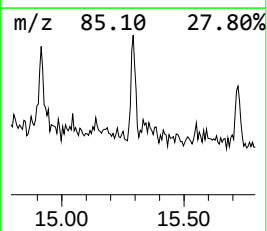
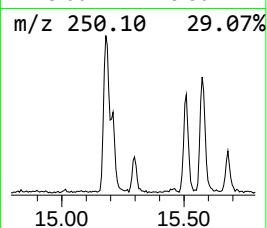
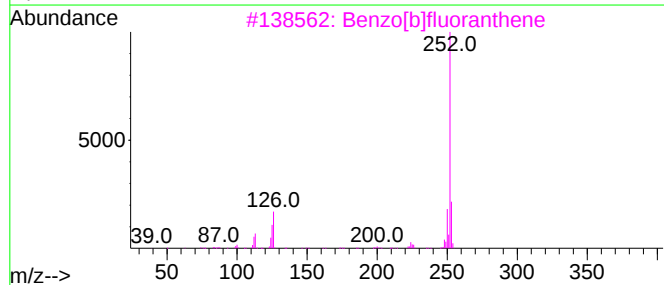
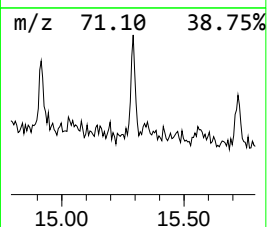
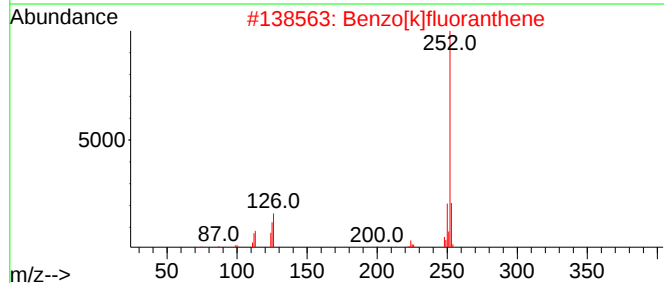
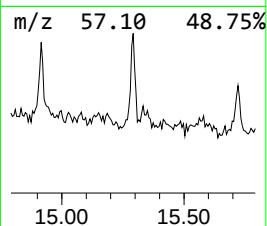
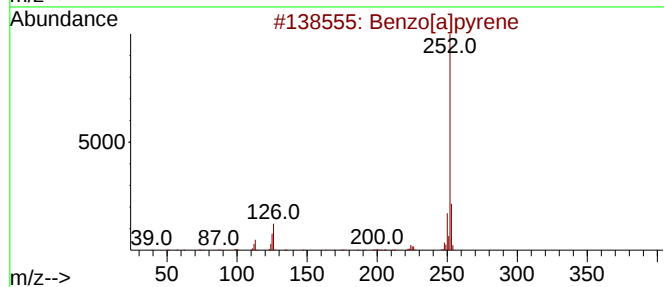
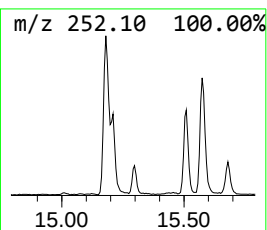
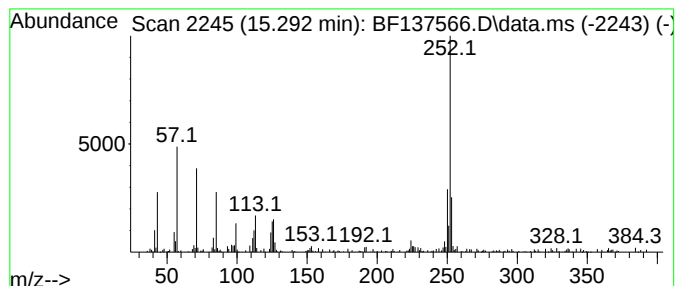
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Benzo[j]fluoranthene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.292	2.52 ng	123676	Perylene-d12	15.645

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[a]pyrene	252	C20H12	000050-32-8	94
2			Benzo[k]fluoranthene	252	C20H12	000207-08-9	92
3			Benzo[b]fluoranthene	252	C20H12	000205-99-2	89
4			Benzo[j]fluoranthene	252	C20H12	000205-82-3	70
5			Benzo[e]pyrene	252	C20H12	000192-97-2	70



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF031124\
Data File : BF137566.D
Acq On : 11 Mar 2024 20:18
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Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RCA-1-COMP

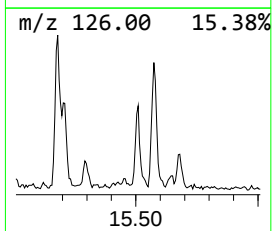
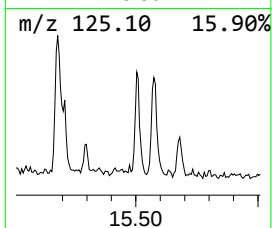
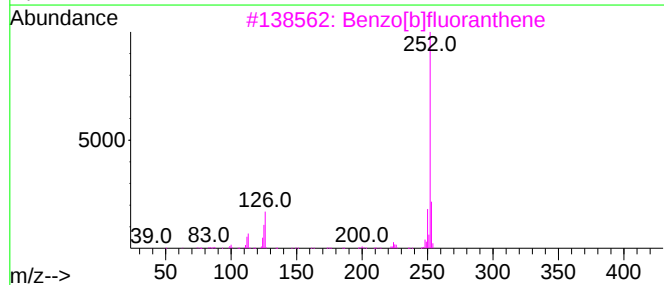
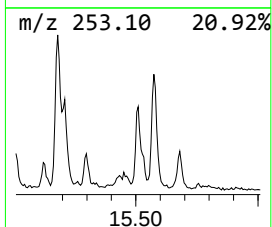
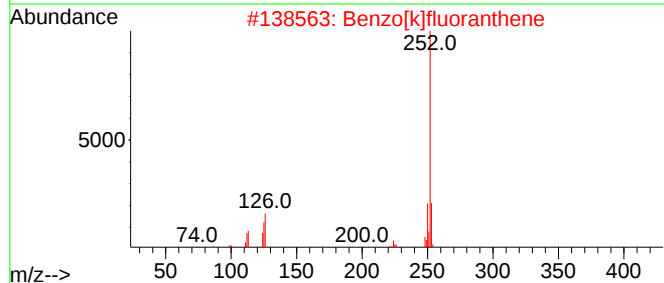
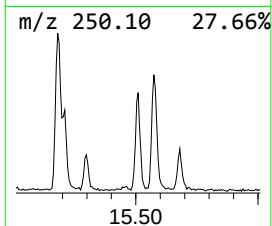
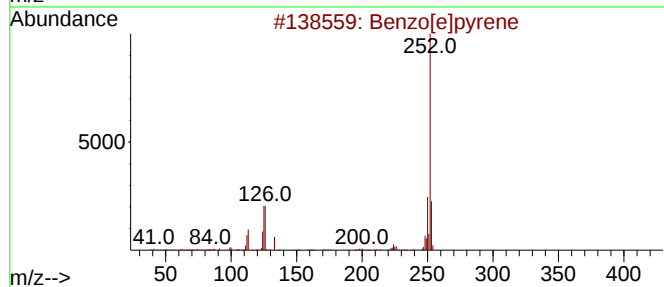
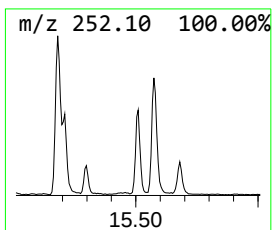
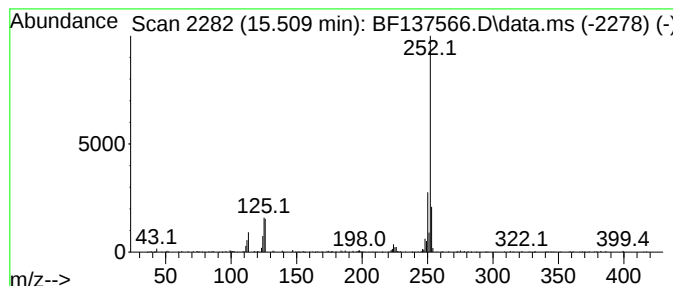
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Benzo[e]pyrene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.509	5.26 ng	258406	Perylene-d12	15.645

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[e]pyrene	252	C20H12	000192-97-2	98
2			Benzo[k]fluoranthene	252	C20H12	000207-08-9	97
3			Benzo[b]fluoranthene	252	C20H12	000205-99-2	96
4			Benzo[j]fluoranthene	252	C20H12	000205-82-3	96
5			Perylene	252	C20H12	000198-55-0	94



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF031124\
Data File : BF137566.D
Acq On : 11 Mar 2024 20:18
Operator : CG\JU
Sample : P1701-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RCA-1-COMP

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022924.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
Butane, 2-metho...	2.263	27.4	ng	1851270	1	6.904	1351230	20.0
Dodecane	10.851	5.4	ng	370901	4	11.427	1371090	20.0
2-Bromo dodecane	11.327	2.3	ng	159601	4	11.427	1371090	20.0
1-Pentadecene	11.669	3.0	ng	202894	4	11.427	1371090	20.0
n-Hexadecanoic ...	11.974	3.5	ng	242389	4	11.427	1371090	20.0
Isopropyl palmi...	12.221	2.9	ng	196592	4	11.427	1371090	20.0
unknown12.527	12.527	2.9	ng	198588	4	11.427	1371090	20.0
Tricosyl heptaf...	13.951	3.7	ng	304346	5	14.092	1647550	20.0
3,7,11-Trimethy...	14.998	2.6	ng	129499	6	15.645	982748	20.0
Benzo[j]fluoran...	15.292	2.5	ng	123676	6	15.645	982748	20.0
Benzo[e]pyrene	15.509	5.3	ng	258406	6	15.645	982748	20.0