

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF121718\
 Data File : BF111565.D
 Acq On : 18 Dec 2018 3:21
 Operator : JU/SJ
 Sample : J6403-57
 Misc :
 ALS Vial : 26 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP-8-A

Integration Parameters: rteint.p
 Integrator: RTE
 Smoothing : ON
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0
 Filtering: 5
 Min Area: 3 % of largest Peak
 Max Peaks: 100
 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-BF121418.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.252	195	198	215	rBV	21068	72632	3.18%	0.353%
2	4.993	489	494	502	rBV	91981	110406	4.84%	0.536%
3	5.422	563	567	582	rBV	2214111	2021810	88.60%	9.816%
4	6.434	735	739	757	rBV	2129845	2281983	100.00%	11.079%
5	6.563	757	761	764	rBV	2550430	2134850	93.55%	10.365%
6	6.787	795	799	803	rBV	857778	686701	30.09%	3.334%
7	6.945	822	826	829	rBV	1995441	1600494	70.14%	7.770%
8	7.345	889	894	897	rBV	1421654	1309891	57.40%	6.360%
9	8.069	1013	1017	1024	rBV	1011004	868852	38.07%	4.218%
10	9.145	1196	1200	1203	rBV	2630954	2081163	91.20%	10.104%
11	9.539	1263	1267	1274	rBV	173020	158126	6.93%	0.768%
12	9.822	1311	1315	1326	rVB	978843	902860	39.56%	4.383%
13	10.610	1445	1449	1463	rBV	1197096	1083171	47.47%	5.259%
14	11.310	1564	1568	1570	rBV	742519	710353	31.13%	3.449%
15	11.327	1570	1571	1578	rVB	107510	85381	3.74%	0.415%
16	11.839	1655	1658	1661	rBV	119275	108071	4.74%	0.525%
17	12.516	1770	1773	1778	rBV	139795	136138	5.97%	0.661%
18	12.621	1788	1791	1796	rBV6	25971	34845	1.53%	0.169%
19	12.745	1807	1812	1815	rBV	142651	133985	5.87%	0.650%
20	12.892	1833	1837	1840	rBV	1707922	1445495	63.34%	7.018%
21	13.468	1930	1935	1938	rBV4	29224	29232	1.28%	0.142%
22	13.798	1987	1991	1996	rBV2	80791	96085	4.21%	0.466%
23	13.945	2011	2016	2019	rBV	749017	750284	32.88%	3.643%
24	13.968	2019	2020	2029	rVB	92594	72796	3.19%	0.353%
25	14.116	2042	2045	2051	rVB	71150	64220	2.81%	0.312%
26	14.421	2094	2097	2100	rVB	118119	103087	4.52%	0.500%
27	14.721	2145	2148	2151	rVB	120287	120166	5.27%	0.583%
28	14.792	2157	2160	2165	rVB	66751	68708	3.01%	0.334%
29	14.968	2186	2190	2200	rBV2	65793	129436	5.67%	0.628%
30	15.045	2200	2203	2207	rBV	154275	171632	7.52%	0.833%
31	15.262	2236	2240	2246	rVB	37705	53733	2.35%	0.261%
32	15.321	2247	2250	2254	rVB	44055	52384	2.30%	0.254%
33	15.380	2256	2260	2264	rBV	374742	514365	22.54%	2.497%
34	15.415	2264	2266	2271	rVB	142358	156514	6.86%	0.760%

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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

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35	15.839	2333	2338	2343	rVB	101530	163870	7.18%	0.796%
36	16.321	2416	2420	2426	rVB2	51631	83539	3.66%	0.406%

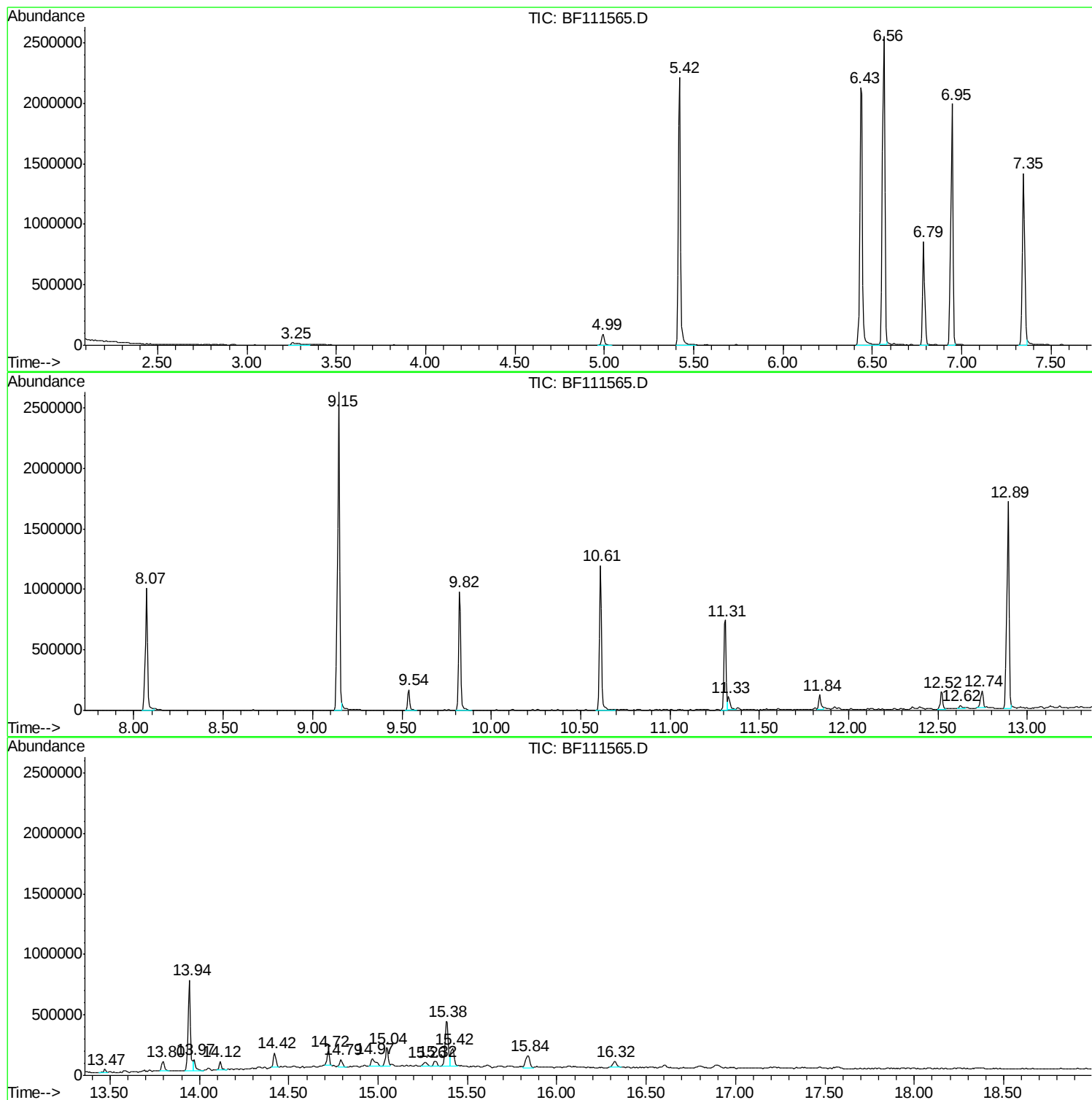
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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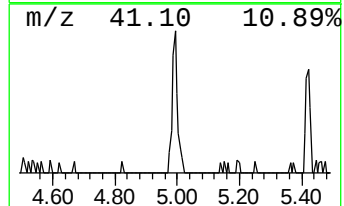
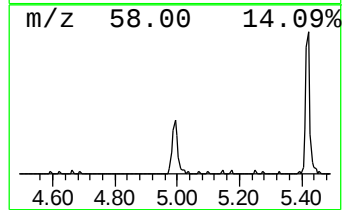
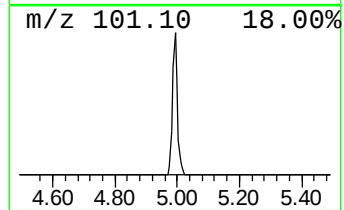
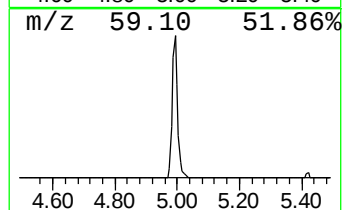
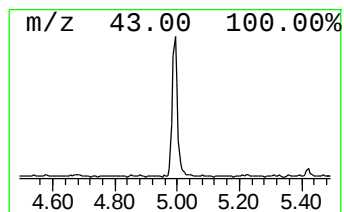
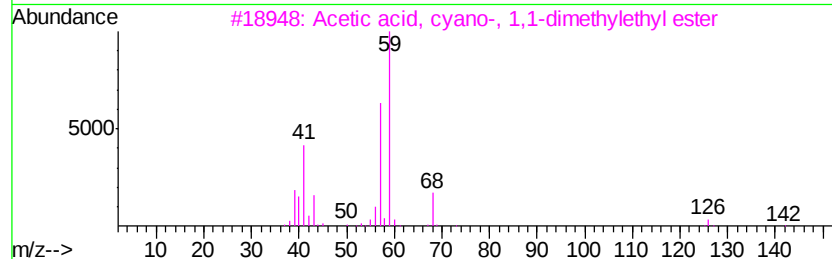
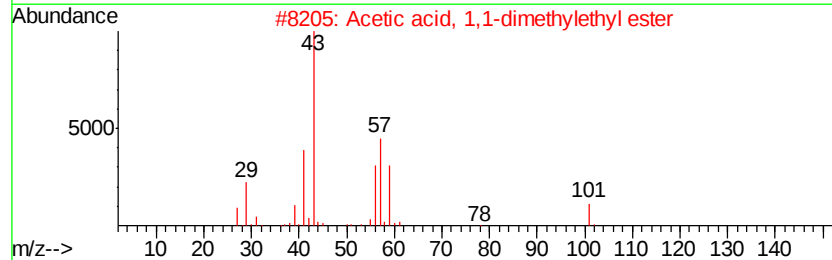
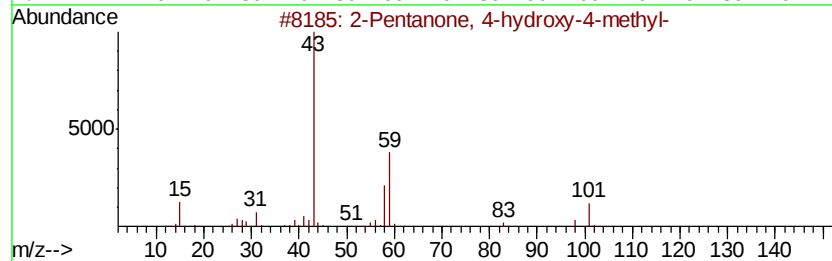
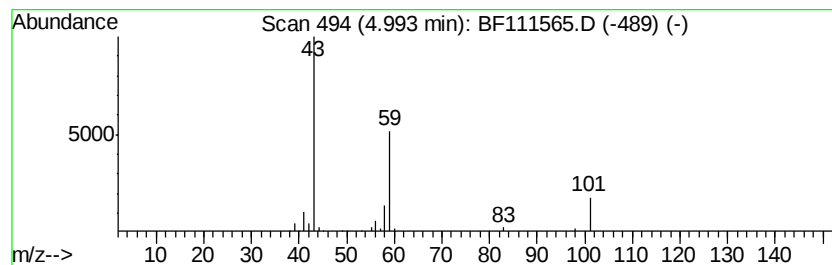
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.99	3.22 ng	110406	1,4-Dichlorobenzene-d4	6.79

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-			116	C6H12O2	000123-42-2	40
2	Acetic acid, 1,1-dimethylethyl e...			116	C6H12O2	000540-88-5	28
3	Acetic acid, cyano-, 1,1-dimethv...			141	C7H11NO2	001116-98-9	25
4	4-Penten-2-one, 4-methyl-			98	C6H10O	003744-02-3	9
5	2,3-Butanedione, monooxime			101	C4H7NO2	000057-71-6	9



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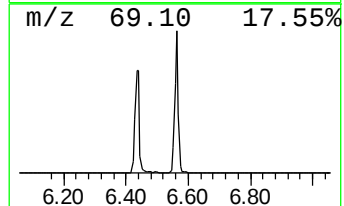
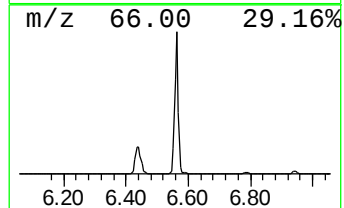
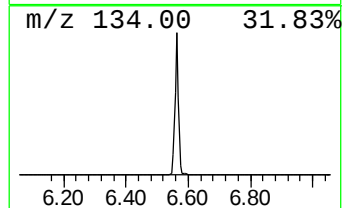
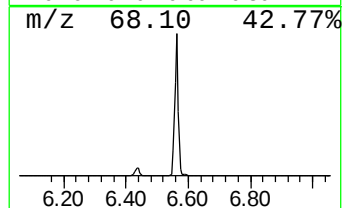
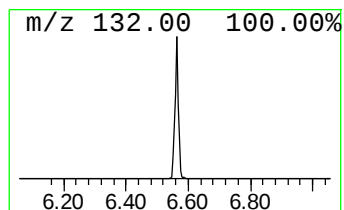
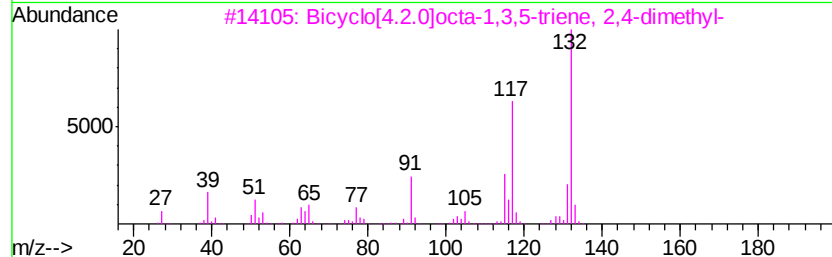
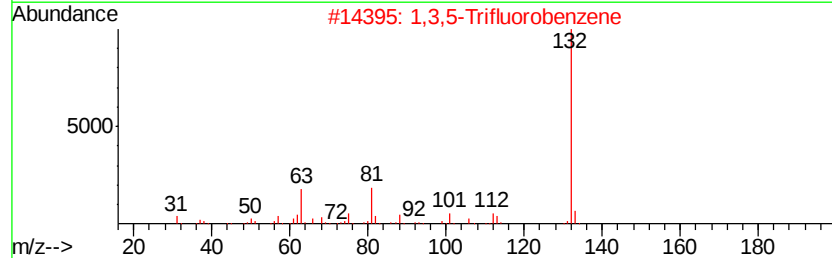
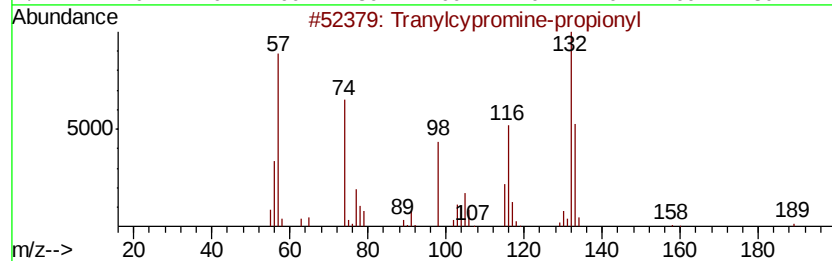
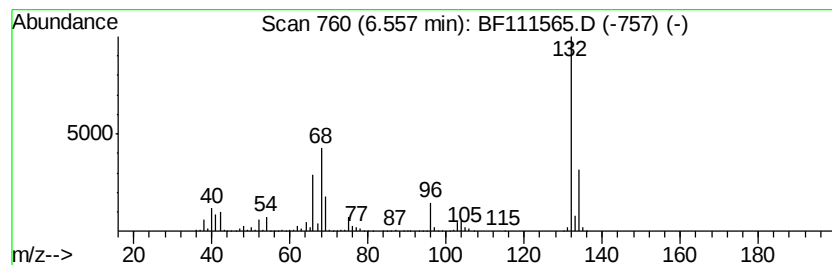
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 3 unknown8.56 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.56	62.18 ng	2134850	1,4-Dichlorobenzene-d4	6.79

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tranvlcvpromine-propionyl	189	C12H15NO	1000123-86-3	12
2		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
3		Bicvclo[4.2.0]octa-1,3,5-triene...	132	C10H12	028749-81-7	9
4		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
5		4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9



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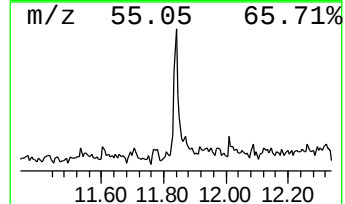
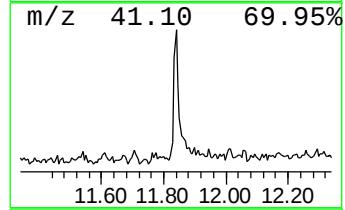
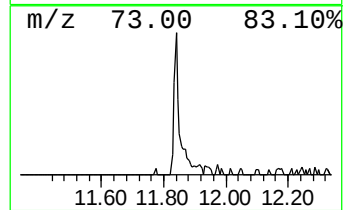
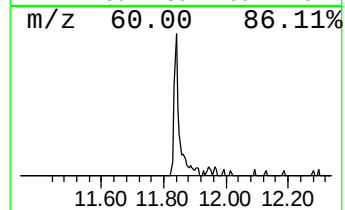
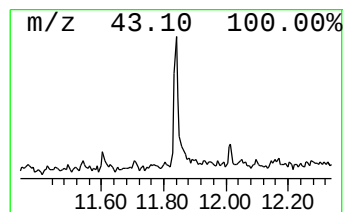
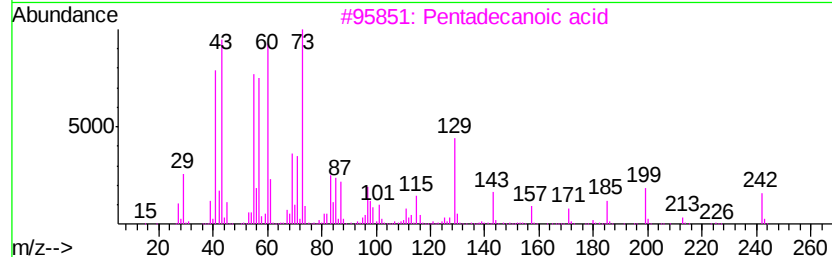
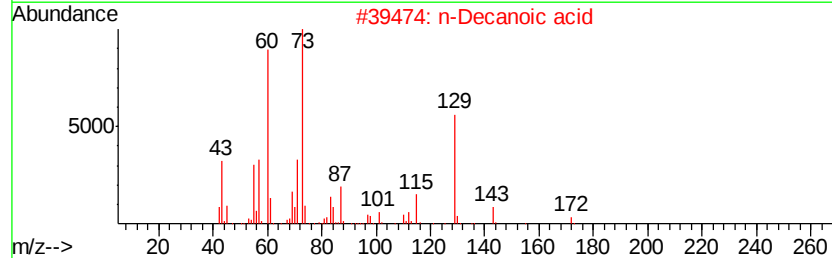
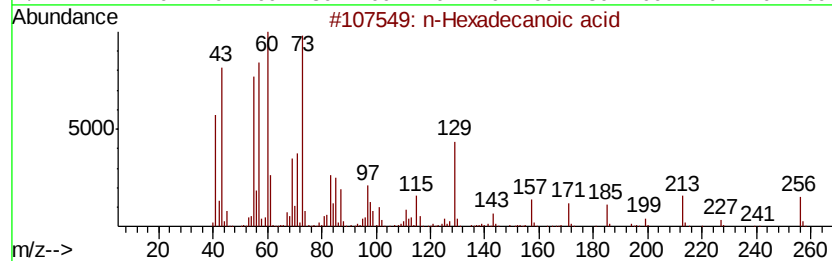
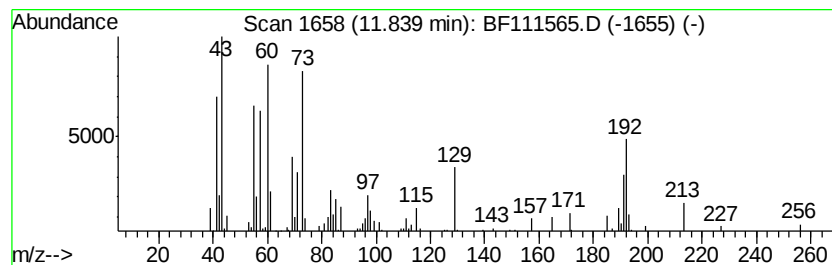
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 n-Hexadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.84	3.04 ng	108071	Phenanthrene-d10	11.31

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	89
2	n-Decanoic acid	172	C10H20O2	000334-48-5	64
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	64
4	Tridecanoic acid	214	C13H26O2	000638-53-9	52
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	50



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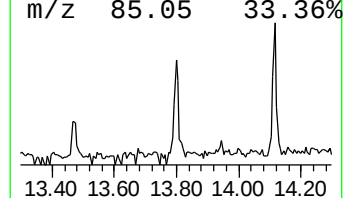
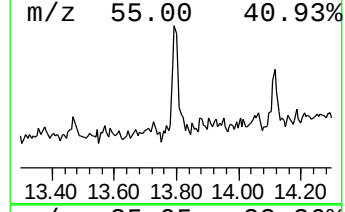
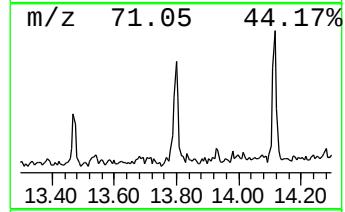
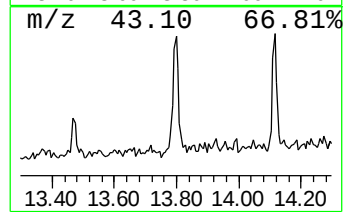
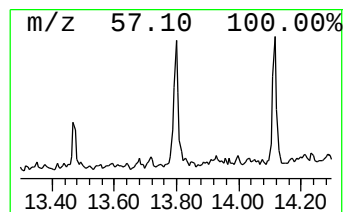
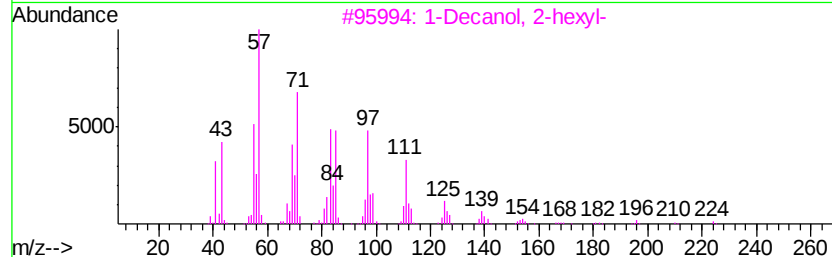
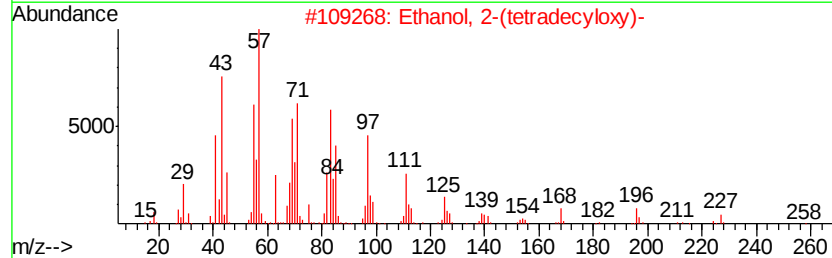
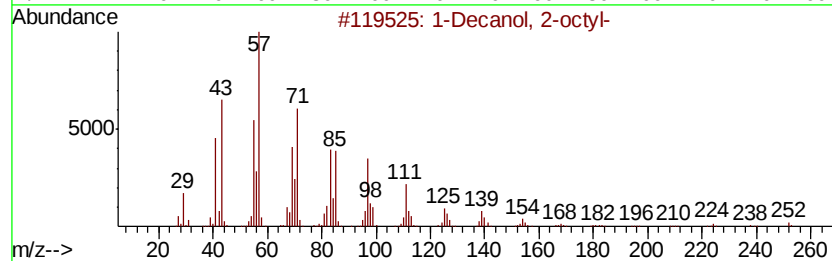
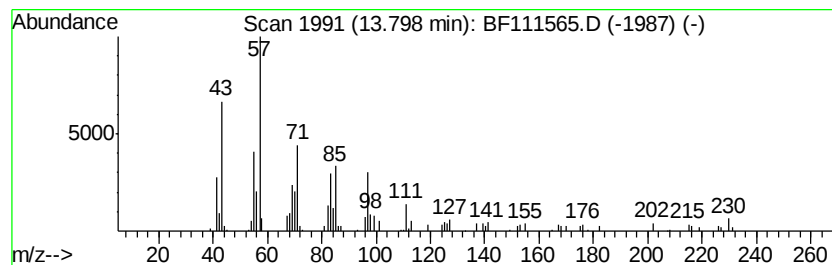
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 1-Decanol, 2-octyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.80	2.56 ng	96085	Chrysene-d12	13.94

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Decanol, 2-octyl-	270	C18H38O	045235-48-1	86
2		Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	86
3		1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	86
4		Oxirane, [(dodecyloxy)methyl]-	242	C15H30O2	002461-18-9	72
5		Hexadecane	226	C16H34	000544-76-3	60



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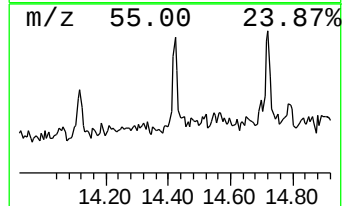
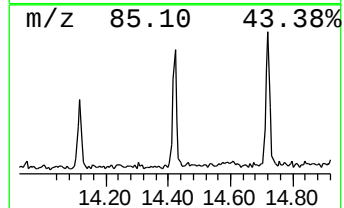
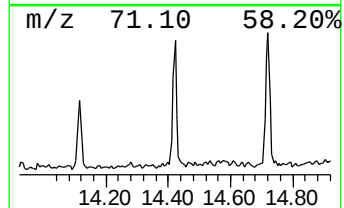
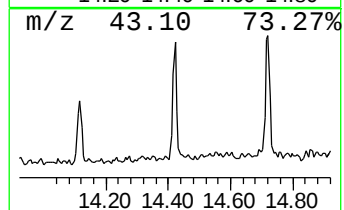
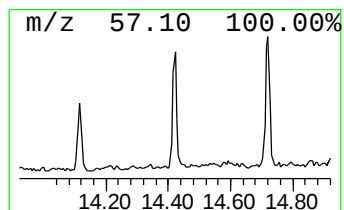
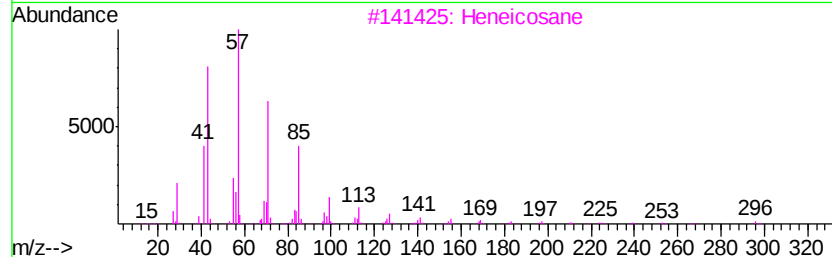
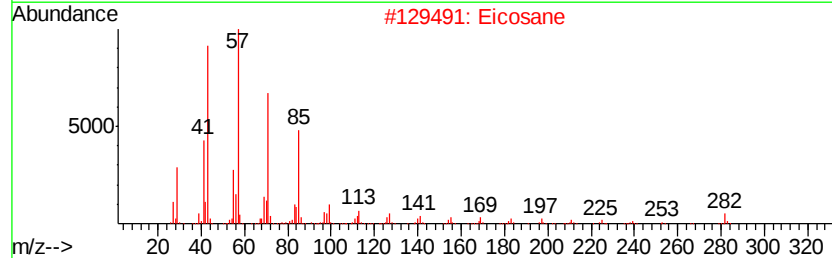
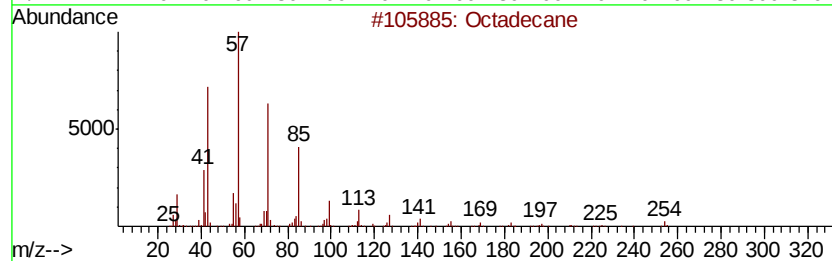
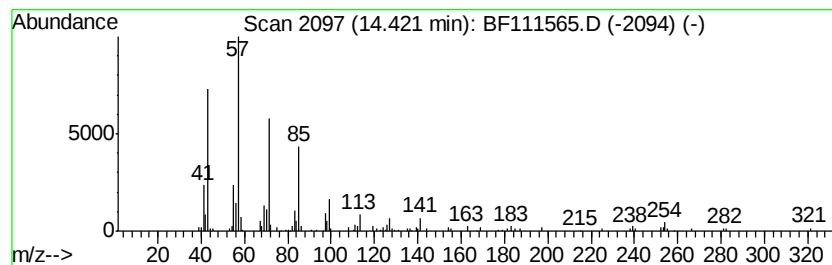
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 Peak Number 7 Octadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.42	2.75 ng	103087	Chrysene-d12	13.94

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane		254	C18H38	000593-45-3	93
2	Eicosane		282	C20H42	000112-95-8	93
3	Heneicosane		296	C21H44	000629-94-7	87
4	Pentacosane		352	C25H52	000629-99-2	87
5	Docosane, 11-butyl-		366	C26H54	013475-76-8	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121718\
Data File : BF111565.D
Acq On : 18 Dec 2018 3:21
Operator : JU/SJ
Sample : J6403-57
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-8-A

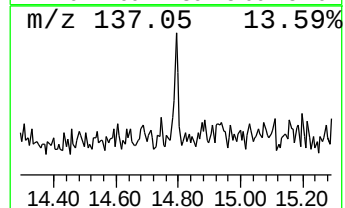
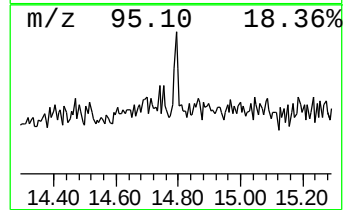
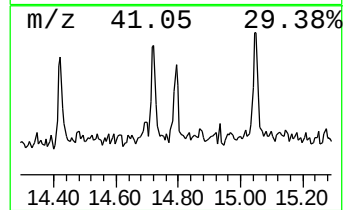
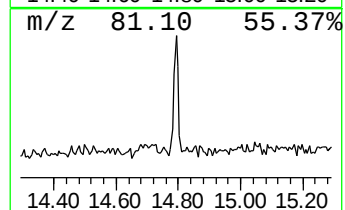
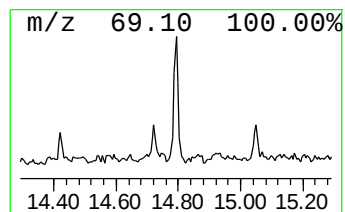
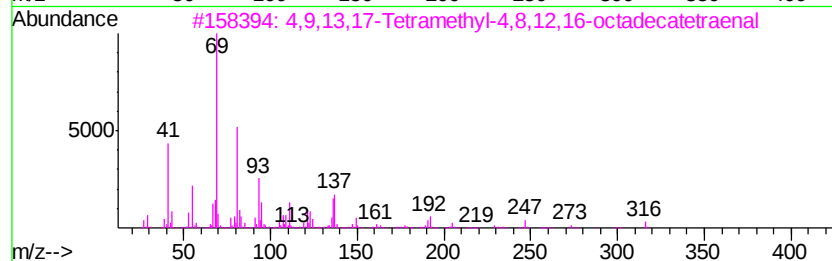
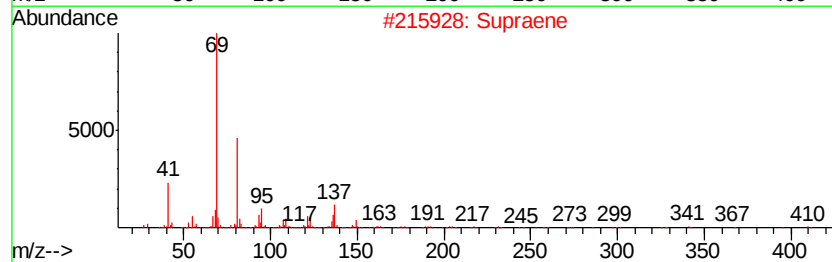
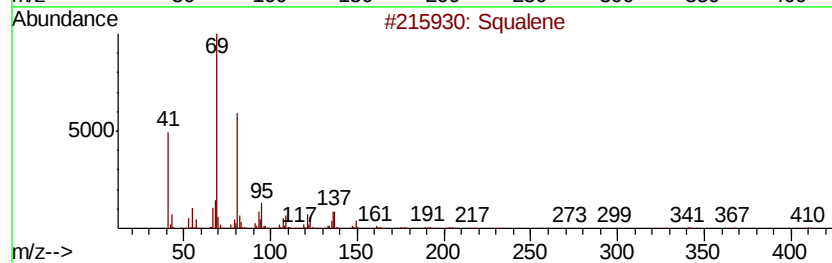
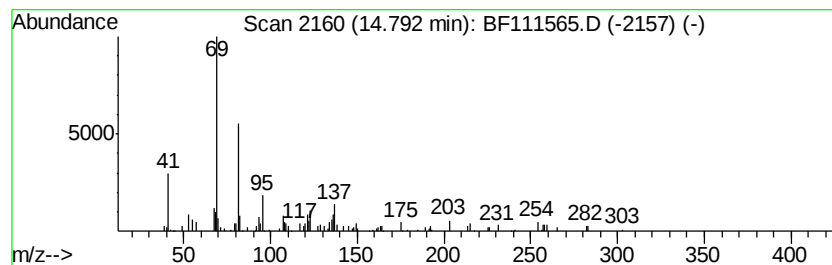
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 Squalene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.79	2.67 ng	68708	Perylene-d12	15.38

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Squalene	410	C30H50	000111-02-4	80
2		Supraene	410	C30H50	007683-64-9	80
3		4,9,13,17-Tetramethyl-4,8,12,16-...	316	C22H36O	056882-09-8	72
4		4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	72
5		2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	004602-84-0	64



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121718\
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Sample : J6403-57
Misc :
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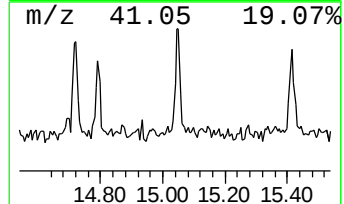
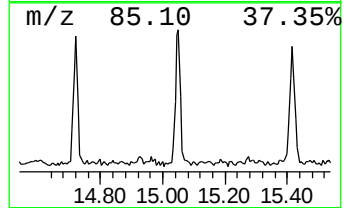
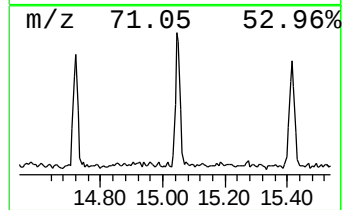
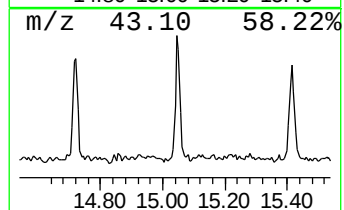
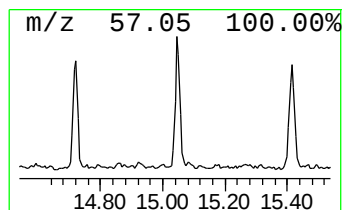
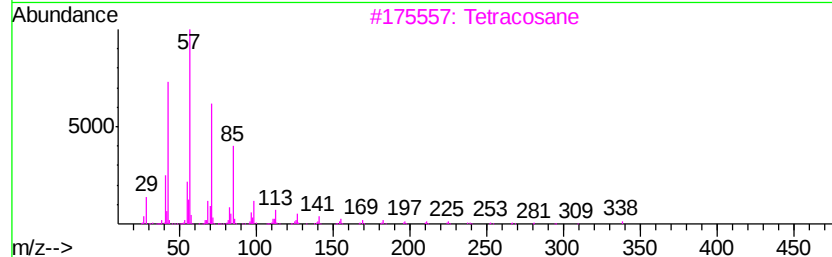
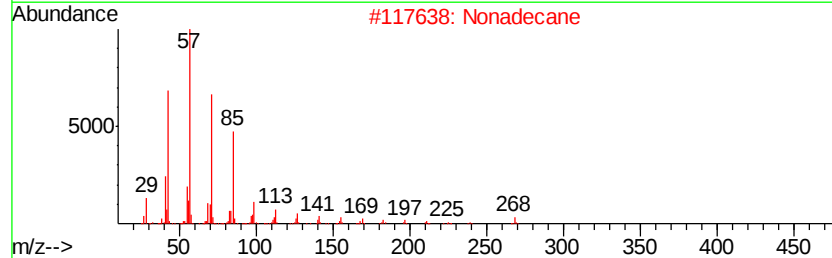
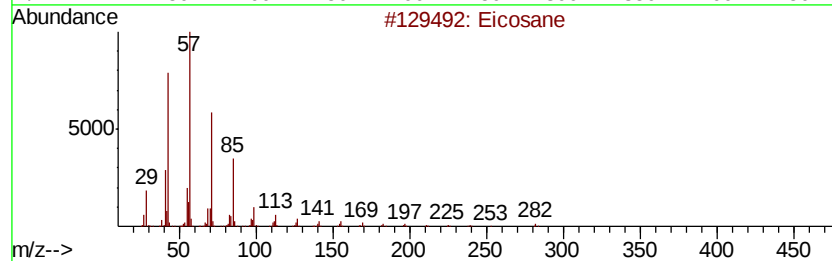
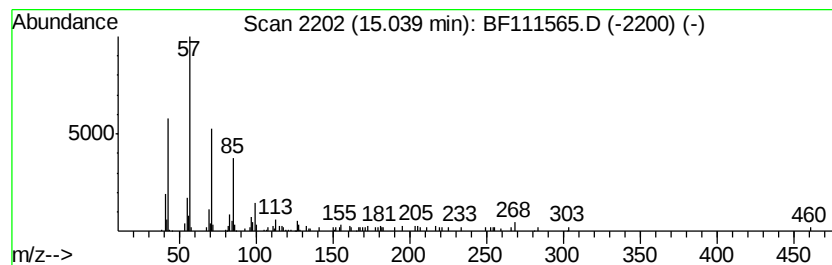
Instrument :
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ClientSampleId :
TP-8-A

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 Eicosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.04	6.67 ng	171632	Perylene-d12	15.38
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Eicosane	282 C20H42	000112-95-8	95
2	Nonadecane	268 C19H40	000629-92-5	93
3	Tetracosane	338 C24H50	000646-31-1	87
4	Heptacosane	380 C27H56	000593-49-7	87
5	Octacosane	394 C28H58	000630-02-4	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121718\
Data File : BF111565.D
Acq On : 18 Dec 2018 3:21
Operator : JU/SJ
Sample : J6403-57
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-8-A

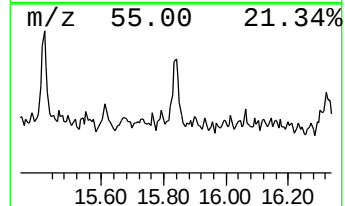
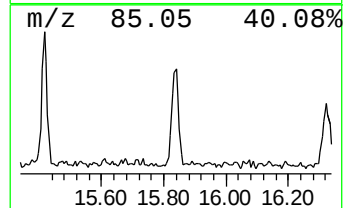
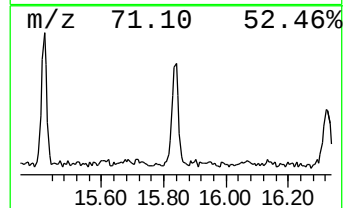
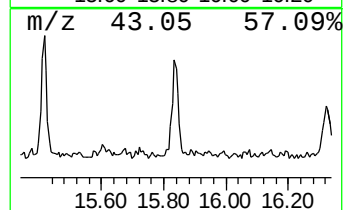
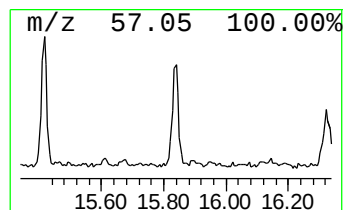
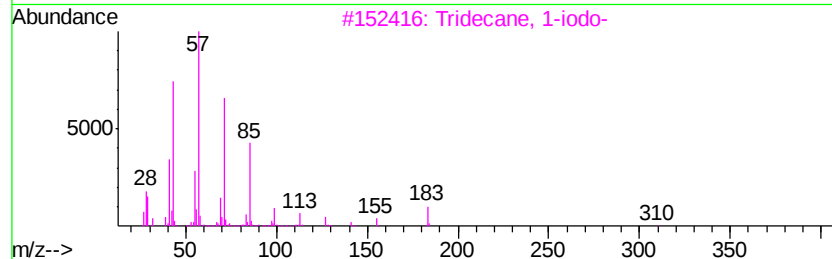
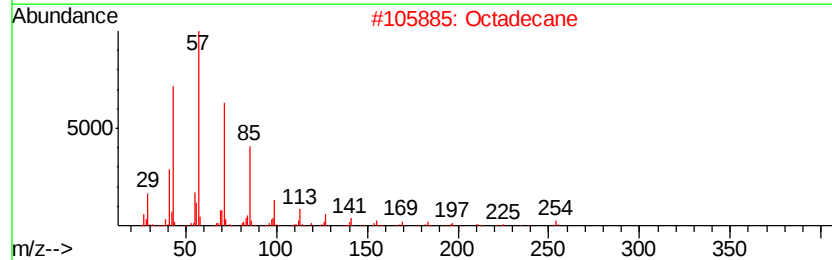
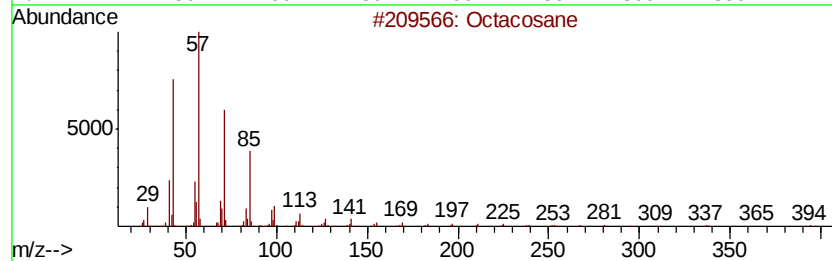
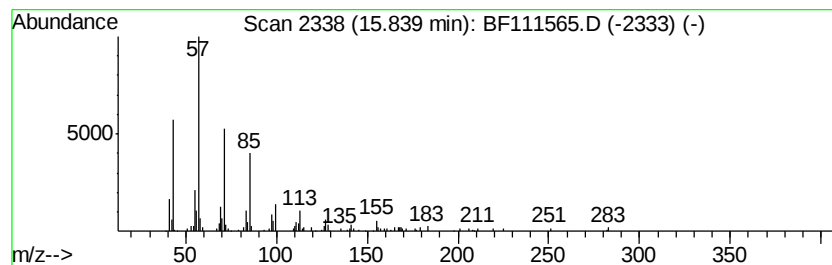
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 12 Octacosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.84	6.37 ng	163870	Perylene-d12	15.38

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octacosane	394	C28H58	000630-02-4	90
2		Octadecane	254	C18H38	000593-45-3	87
3		Tridecane, 1-iodo-	310	C13H27I	035599-77-0	87
4		Hexacosane	366	C26H54	000630-01-3	87
5		Hentriacontane	437	C31H64	000630-04-6	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121718\
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Operator : JU/SJ
Sample : J6403-57
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-8-A

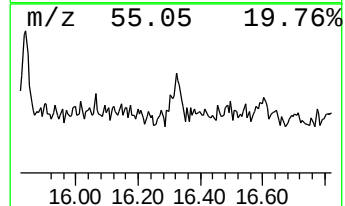
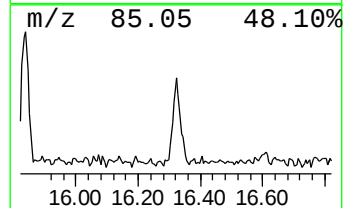
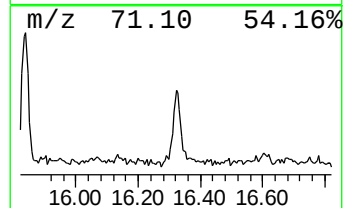
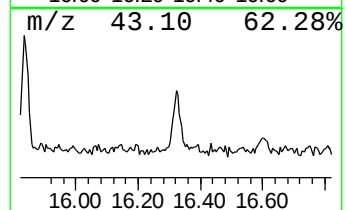
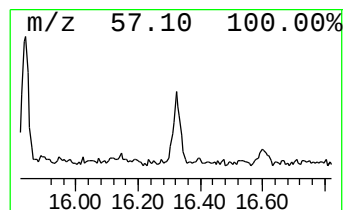
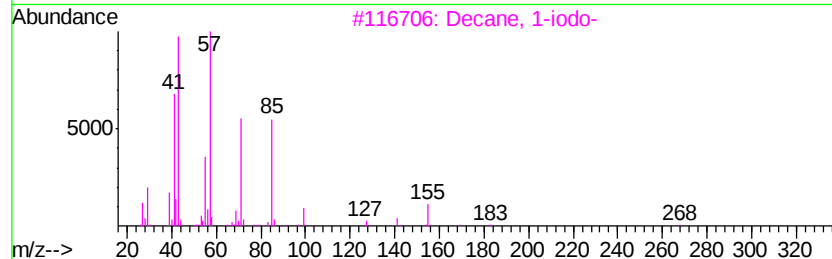
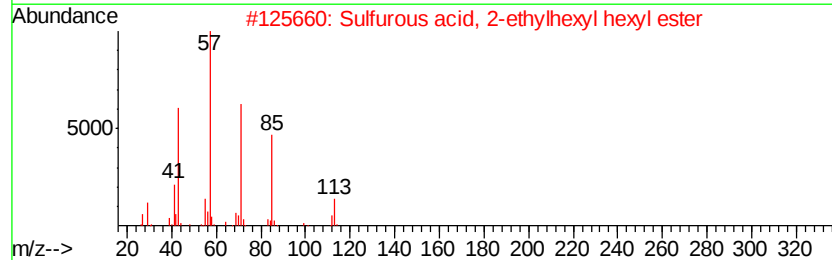
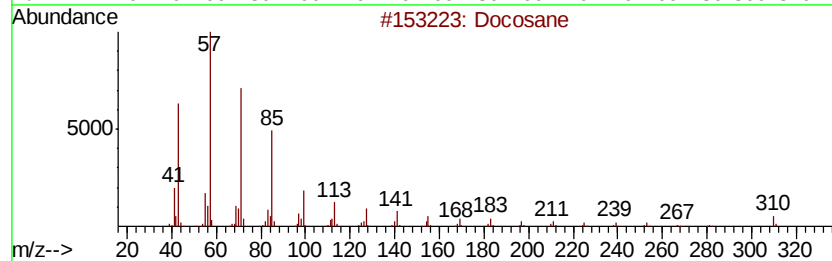
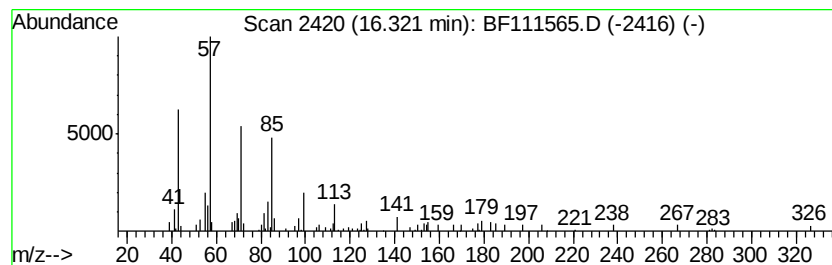
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 13 Docosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.32	3.25 ng	83539	Perylene-d12	15.38

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Docosane	310	C22H46	000629-97-0	86
2		Sulfurous acid, 2-ethylhexyl hex...	278	C14H30O3S	1000309-20-2	59
3		Decane, 1-iodo-	268	C10H21I	002050-77-3	53
4		5,5-Dibutylnonane	240	C17H36	006008-17-9	50
5		Sulfurous acid, 2-ethylhexyl iso...	278	C14H30O3S	1000309-19-0	50



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Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-8-A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF121418.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.99	3.2	ng	110406	1	6.79	686701	20.0
unknown8.56	6.56	62.2	ng	2134850	1	6.79	686701	20.0
n-Hexadecanoic acid	11.84	3.0	ng	108071	4	11.31	710353	20.0
1-Decanol, 2-octyl-	13.80	2.6	ng	96085	5	13.94	750284	20.0
Octadecane	14.42	2.8	ng	103087	5	13.94	750284	20.0
Squalene	14.79	2.7	ng	68708	6	15.38	514365	20.0
Eicosane	15.04	6.7	ng	171632	6	15.38	514365	20.0
Octacosane	15.84	6.4	ng	163870	6	15.38	514365	20.0
Docosane	16.32	3.3	ng	83539	6	15.38	514365	20.0