

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121718\
 Data File : BF111566.D
 Acq On : 18 Dec 2018 3:48
 Operator : JU/SJ
 Sample : J6403-61
 Misc :
 ALS Vial : 27 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP-8-B

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	3.251	196	198	207	rBV3	24497	49360	1.58%	0.160%
2	4.992	490	494	501	rBV	120430	141911	4.54%	0.459%
3	5.422	563	567	581	rBV	2785035	2542878	81.28%	8.228%
4	6.439	735	740	745	rBV	2685943	2795329	89.35%	9.045%
5	6.563	757	761	764	rBV	3310788	2863679	91.54%	9.266%
6	6.616	767	770	775	rVB2	55126	56121	1.79%	0.182%
7	6.786	795	799	807	rBV	1248934	1014729	32.44%	3.283%
8	6.945	822	826	829	rBV	3004459	2521046	80.58%	8.157%
9	7.345	889	894	907	rBV	2171332	2128448	68.04%	6.887%
10	8.069	1013	1017	1037	rBV	1455818	1313006	41.97%	4.248%
11	9.145	1196	1200	1203	rBV	3734231	3128431	100.00%	10.122%
12	9.539	1263	1267	1280	rBV	417546	378017	12.08%	1.223%
13	9.822	1311	1315	1326	rVB2	1361645	1249229	39.93%	4.042%
14	10.610	1445	1449	1460	rBV	1657143	1551742	49.60%	5.021%
15	10.733	1463	1470	1479	rVB7	22582	47191	1.51%	0.153%
16	11.304	1564	1567	1570	rBV	978185	953237	30.47%	3.084%
17	11.327	1570	1571	1577	rVB	126593	99606	3.18%	0.322%
18	11.839	1655	1658	1669	rBV2	245822	273086	8.73%	0.884%
19	12.515	1769	1773	1777	rBV	184037	180336	5.76%	0.583%
20	12.621	1788	1791	1797	rBV5	44552	68616	2.19%	0.222%
21	12.745	1807	1812	1815	rBV	175637	168116	5.37%	0.544%
22	12.892	1833	1837	1840	rBV	2461420	2100478	67.14%	6.796%
23	13.127	1875	1877	1882	rVB2	34795	43906	1.40%	0.142%
24	13.368	1915	1918	1924	rVB4	27899	42514	1.36%	0.138%
25	13.468	1930	1935	1938	rBV2	54012	64980	2.08%	0.210%
26	13.792	1986	1990	1998	rBV2	271880	383443	12.26%	1.241%
27	13.945	2011	2016	2019	rBV	1071576	1089855	34.84%	3.526%
28	13.968	2019	2020	2028	rVB	115244	89577	2.86%	0.290%
29	14.115	2042	2045	2051	rVB	149916	124938	3.99%	0.404%
30	14.421	2093	2097	2101	rBV	318342	331639	10.60%	1.073%
31	14.721	2145	2148	2151	rBV	275289	242108	7.74%	0.783%
32	14.792	2157	2160	2164	rVV	121173	112449	3.59%	0.364%
33	14.856	2168	2171	2176	rVB2	59682	61890	1.98%	0.200%
34	14.968	2186	2190	2193	rBV	98484	137392	4.39%	0.445%

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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-BF121418.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	15.051	2200	2204	2207	rBV	345285	380631	12.17%	1.232%
36	15.262	2237	2240	2245	rVB	49844	70938	2.27%	0.230%
37	15.321	2247	2250	2255	rVV	79038	89826	2.87%	0.291%
38	15.380	2255	2260	2263	rVV	593456	756514	24.18%	2.448%
39	15.415	2263	2266	2273	rVB2	306724	377948	12.08%	1.223%
40	15.609	2295	2299	2305	rVB3	96715	129313	4.13%	0.418%
41	15.839	2333	2338	2343	rBV	232467	321326	10.27%	1.040%
42	16.327	2416	2421	2425	rVB	110094	170062	5.44%	0.550%
43	16.603	2463	2468	2473	rBV3	84959	140571	4.49%	0.455%
44	16.898	2513	2518	2524	rVB2	66054	119625	3.82%	0.387%

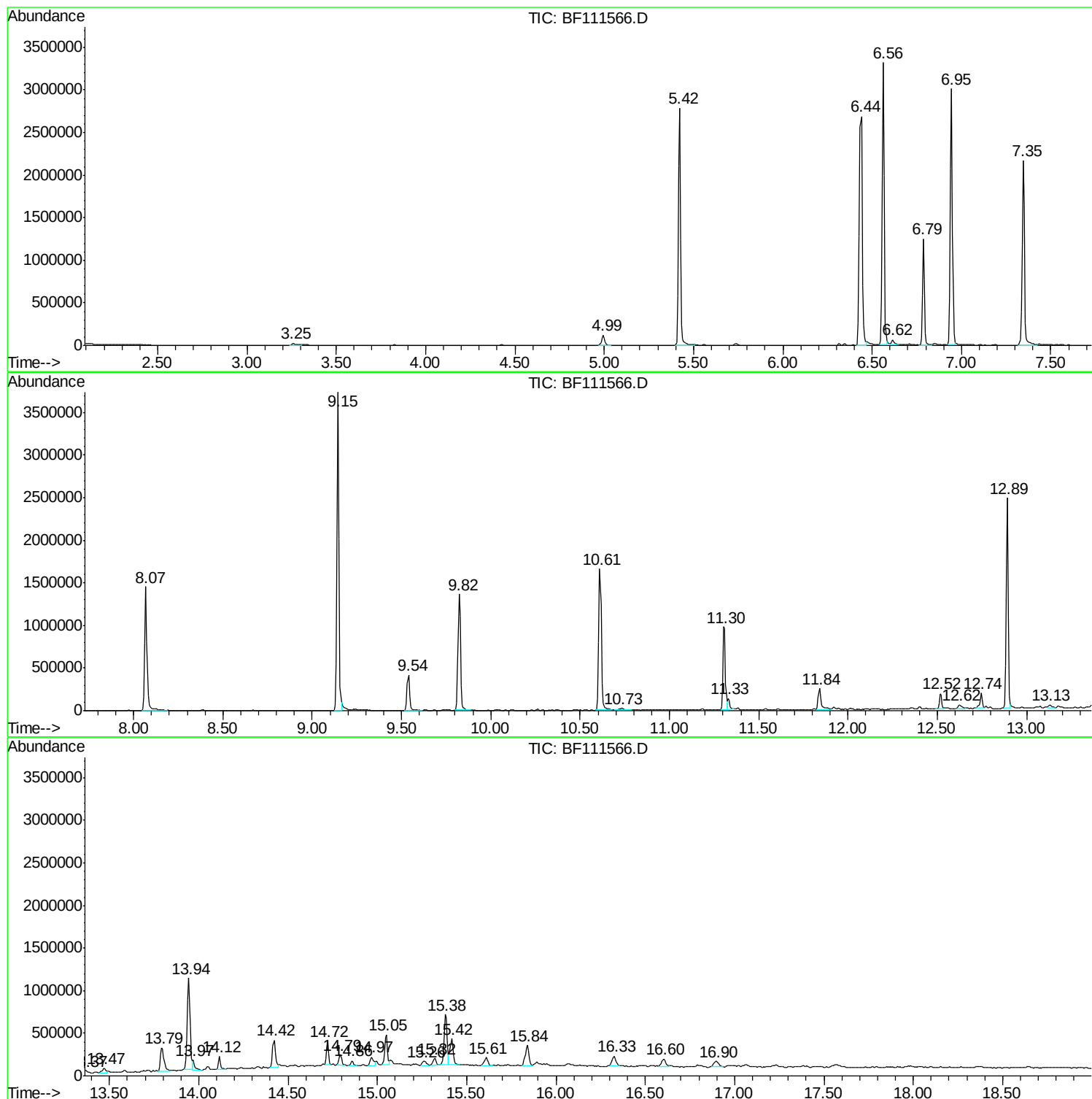
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ClientSampled :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF121418.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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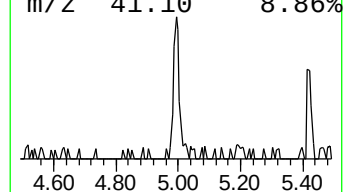
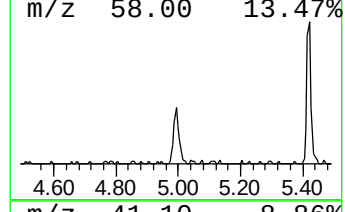
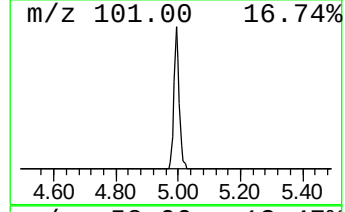
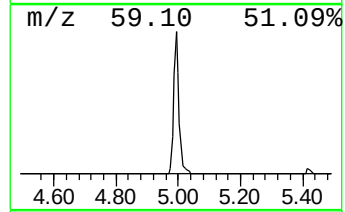
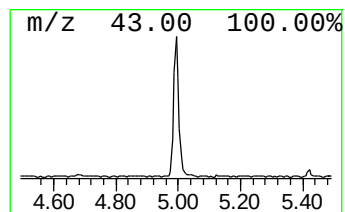
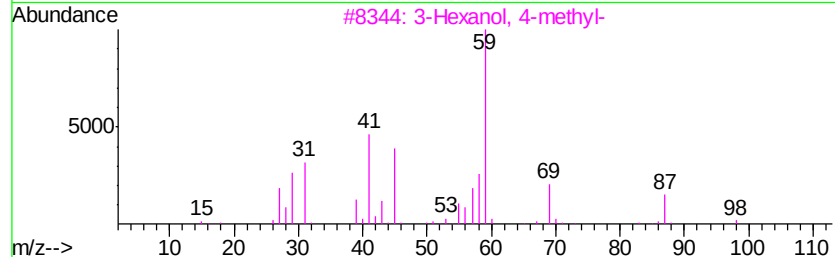
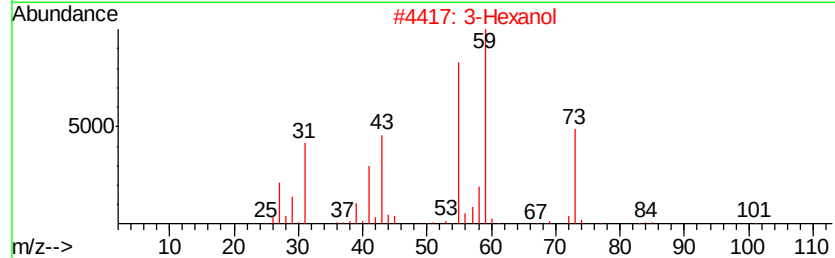
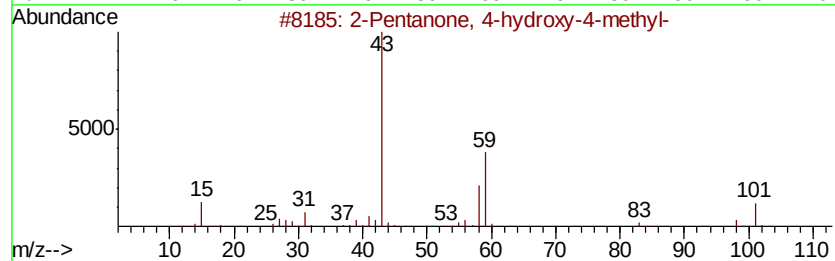
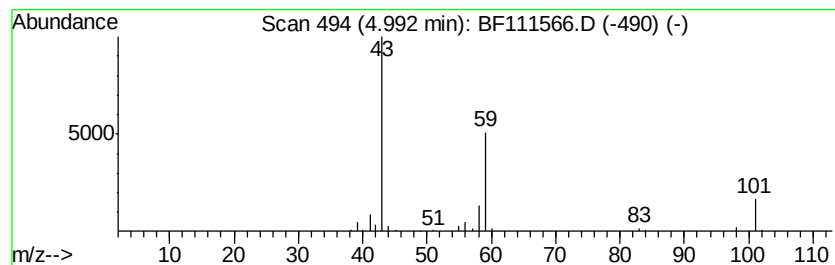
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.99	2.80 ng	141911	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	39
2		3-Hexanol	102	C6H14O	000623-37-0	33
3		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
4		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	27
5		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	25



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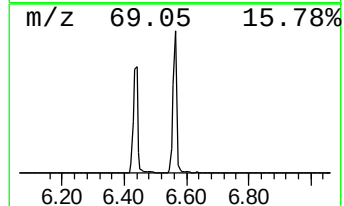
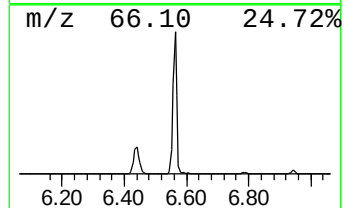
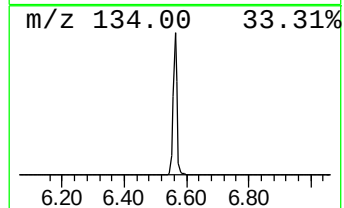
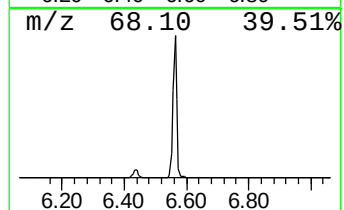
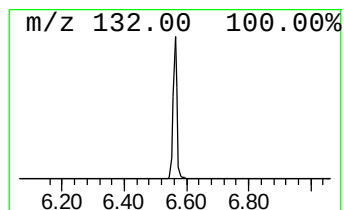
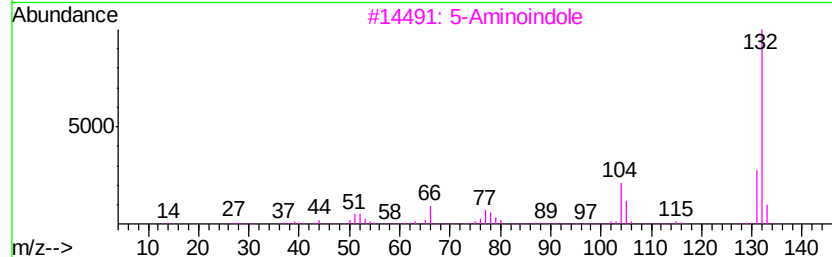
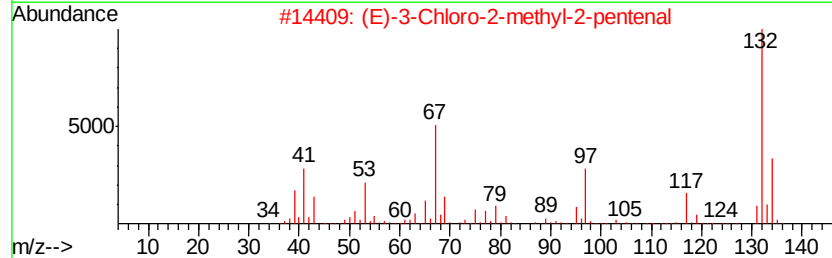
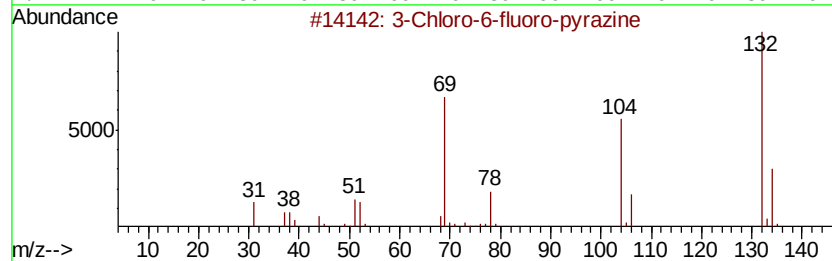
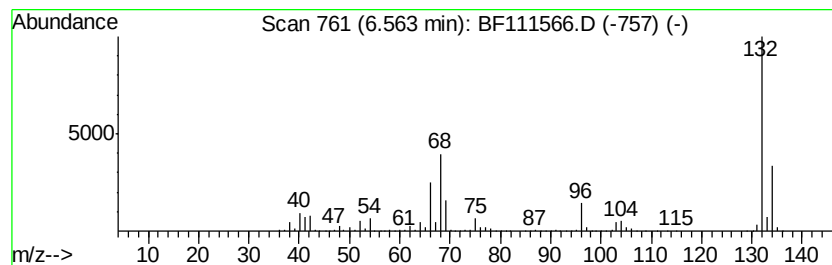
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Peak Number 2 unknown6.56 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.56	56.44 ng	2863680	1,4-Dichlorobenzene-d4	6.79

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9



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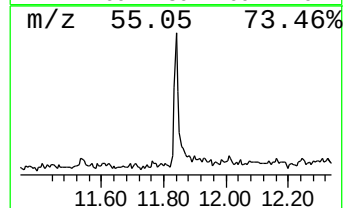
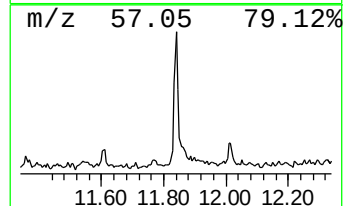
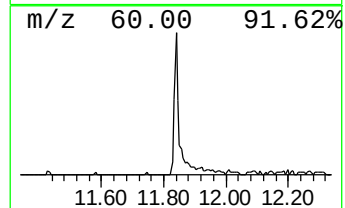
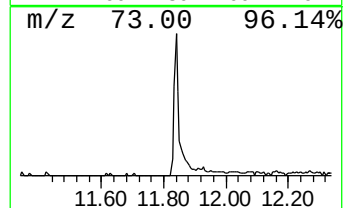
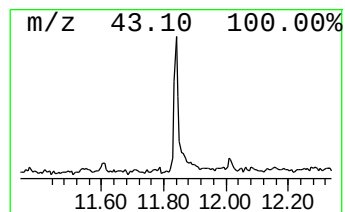
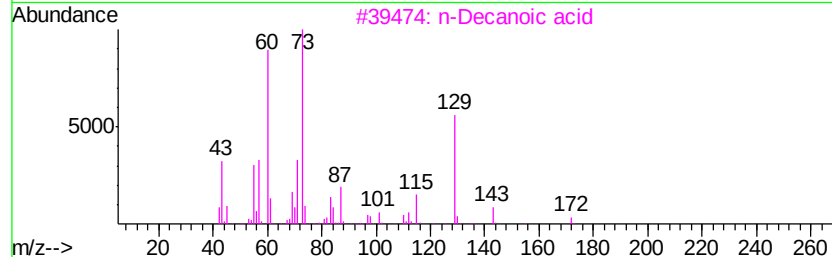
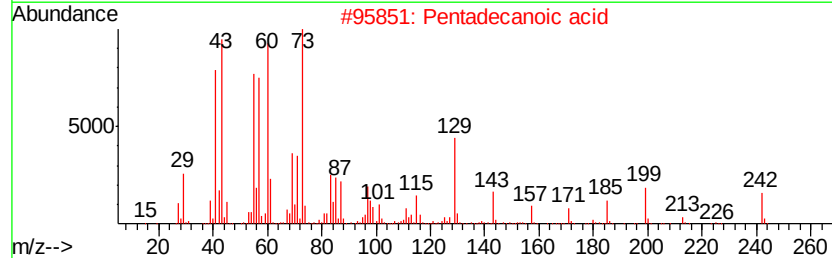
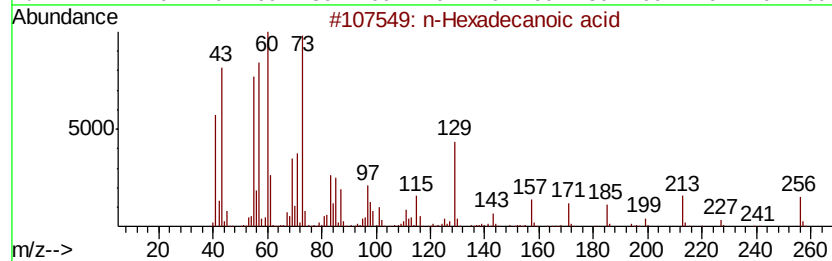
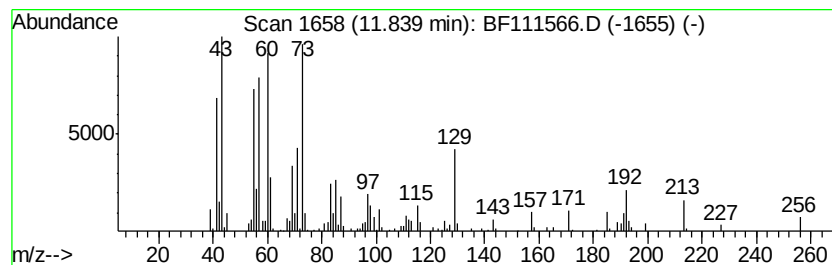
Instrument :
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ClientSampleId :
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Hexadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD		R.T.
11.84	5.73 ng	273086	Phenanthrene-d10		11.31
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	n-Decanoic acid	172	C10H20O2	000334-48-5	86
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5	Tridecanoic acid	214	C13H26O2	000638-53-9	58



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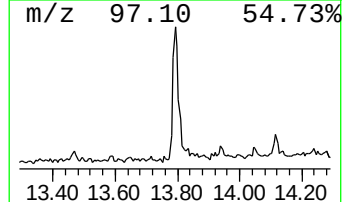
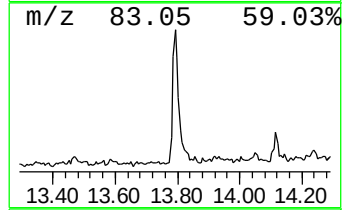
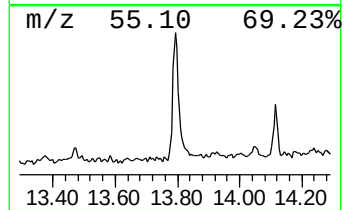
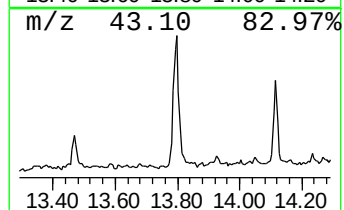
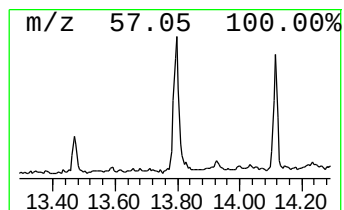
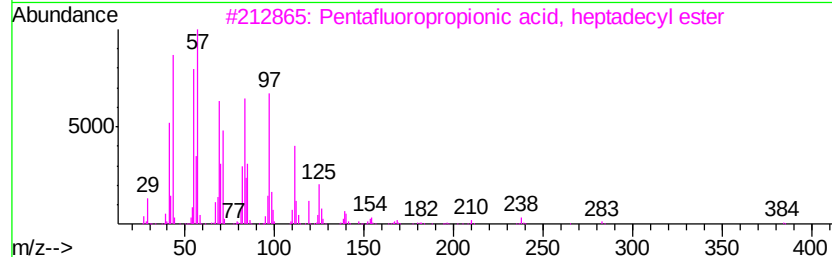
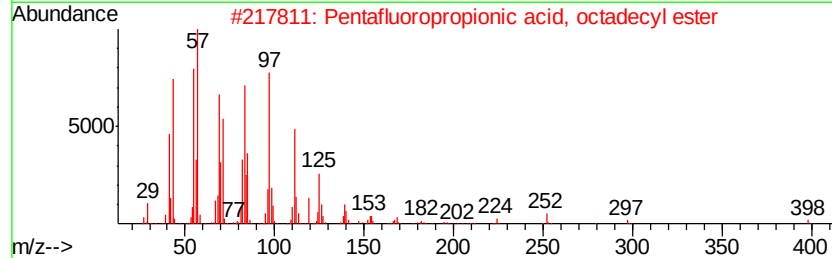
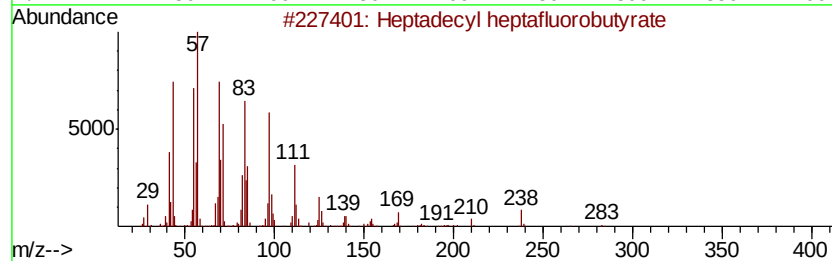
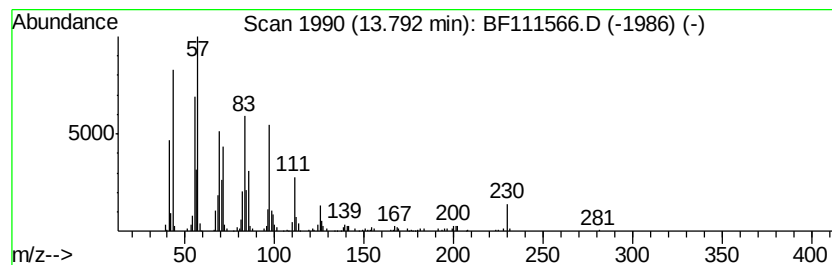
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Heptadecyl heptafluorobutyrate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.79	7.04 ng	383443	Chrysene-d12	13.94

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
2		Pentafluoropropionic acid, octadecyl ester	416	C21H37F5O2	959261-25-7	91
3		Pentafluoropropionic acid, heptadecyl ester	402	C20H35F5O2	959218-78-1	91
4		Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	91
5		Heptafluorobutyric acid, hexadecyl ester	438	C20H33F7O2	006385-15-5	91



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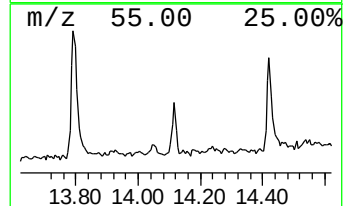
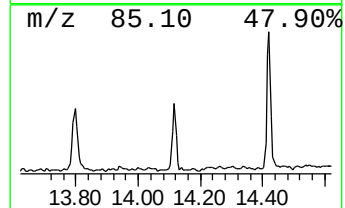
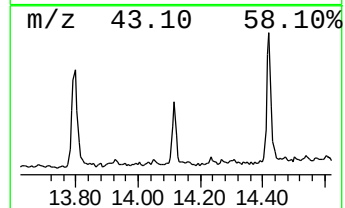
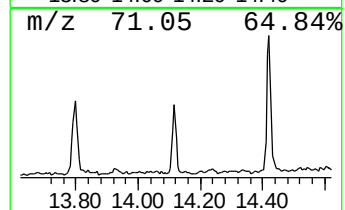
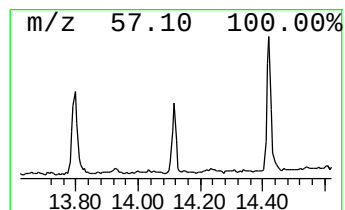
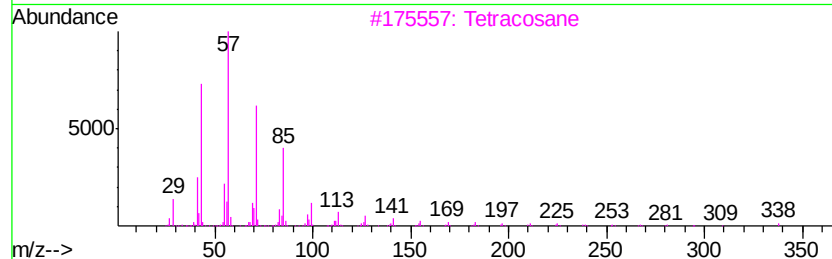
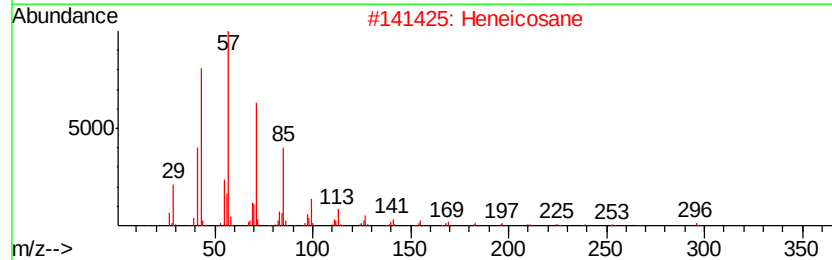
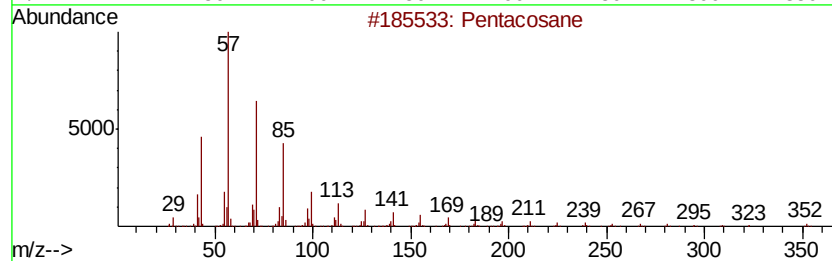
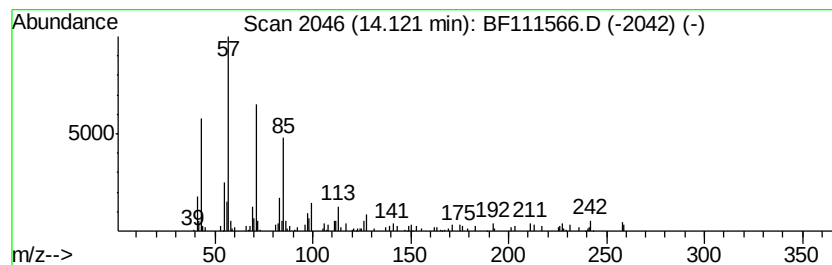
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Pentacosane Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.12	2.29 ng	124938	Chrysene-d12	13.94

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentacosane		352	C25H52	000629-99-2	80
2	Heneicosane		296	C21H44	000629-94-7	80
3	Tetracosane		338	C24H50	000646-31-1	80
4	Eicosane, 9-octyl-		394	C28H58	013475-77-9	80
5	Nonadecane		268	C19H40	000629-92-5	72



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121718\
Data File : BF111566.D
Acq On : 18 Dec 2018 3:48
Operator : JU/SJ
Sample : J6403-61
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-8-B

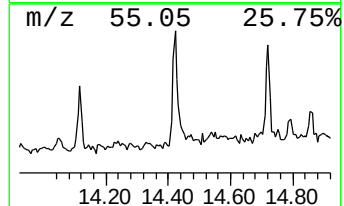
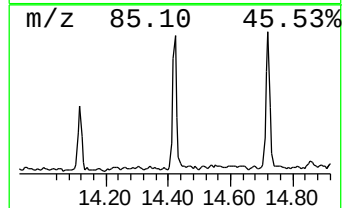
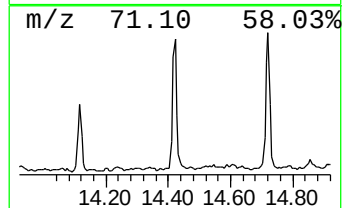
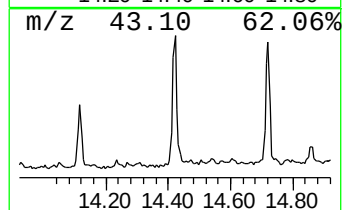
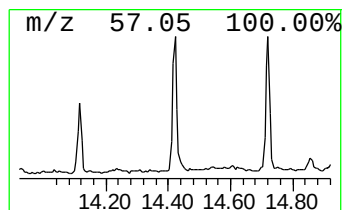
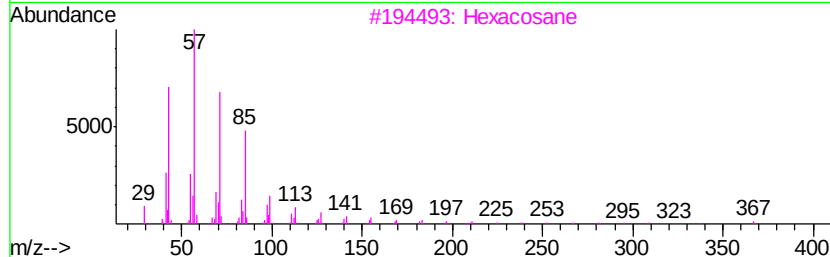
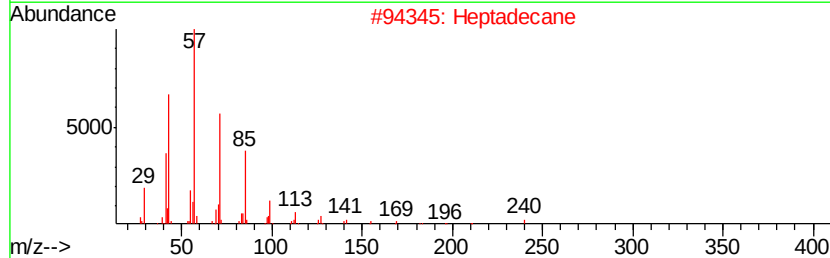
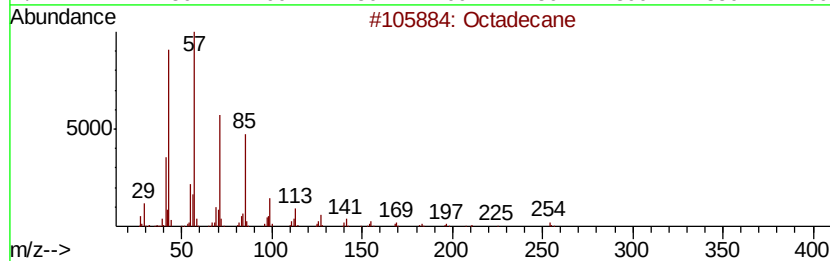
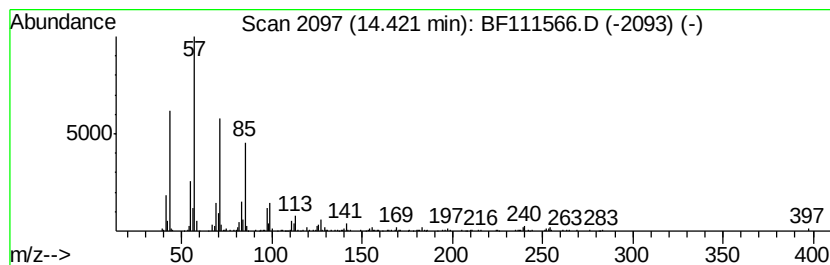
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Octadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.42	6.09 ng	331639	Chrysene-d12	13.94

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecane	254	C18H38	000593-45-3	98
2		Heptadecane	240	C17H36	000629-78-7	96
3		Hexacosane	366	C26H54	000630-01-3	90
4		Hentriacontane	437	C31H64	000630-04-6	90
5		Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121718\
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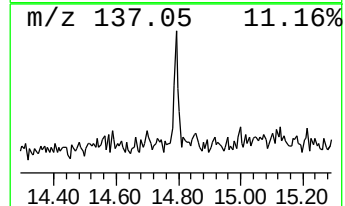
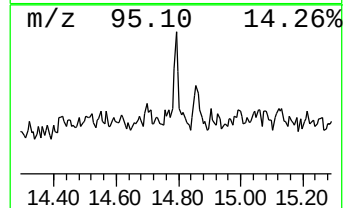
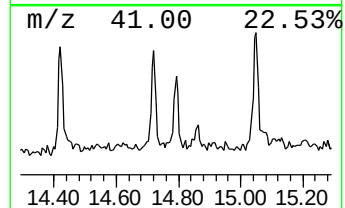
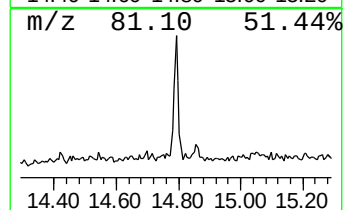
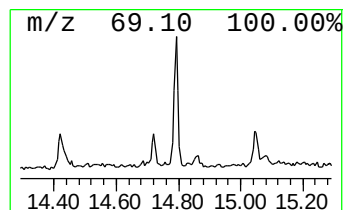
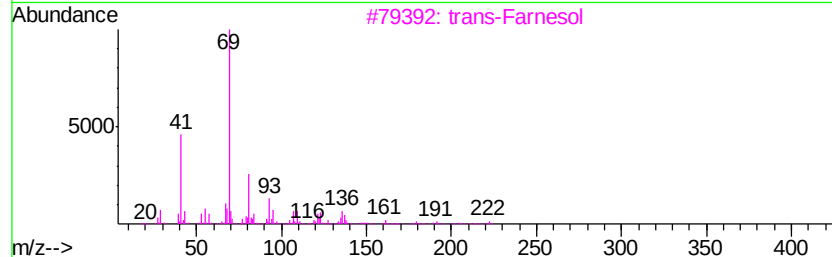
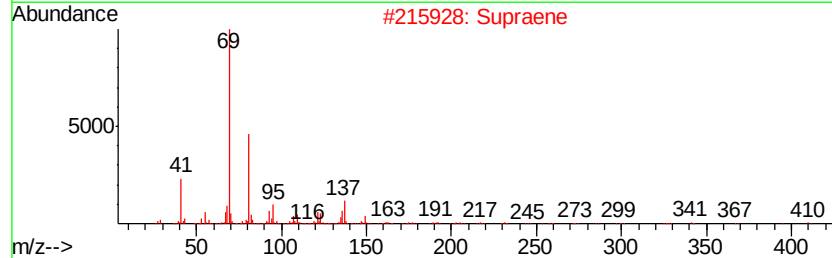
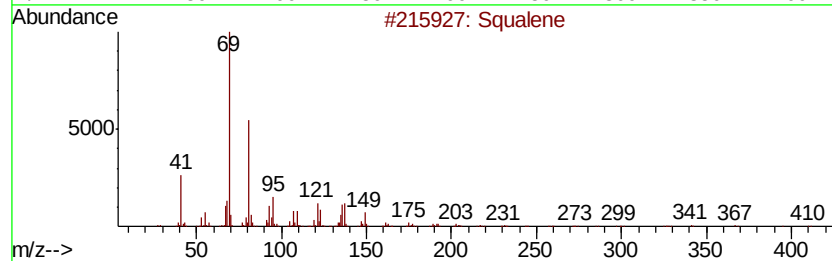
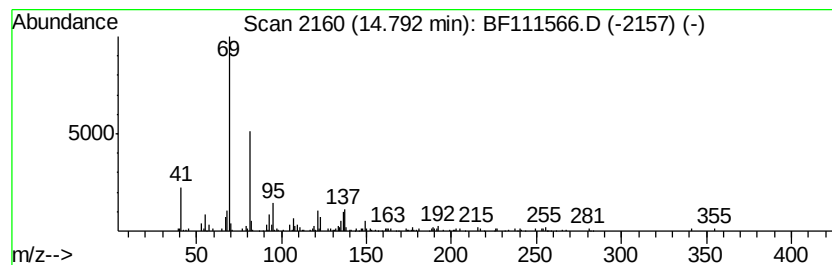
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Squalene Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.79	2.97 ng	112449	Perylene-d12	15.38

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Squalene	410	C30H50	000111-02-4	90
2		Supraene	410	C30H50	007683-64-9	87
3		trans-Farnesol	222	C15H26O	000106-28-5	78
4		2,6,10-Dodecatrien-1-ol, 3,7,11-...	264	C17H28O2	004128-17-0	64
5		2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	004602-84-0	59



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121718\
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ALS Vial : 27 Sample Multiplier: 1

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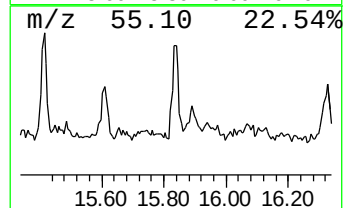
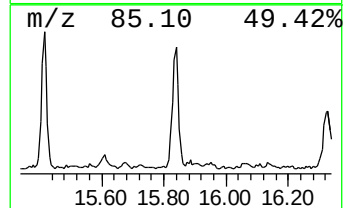
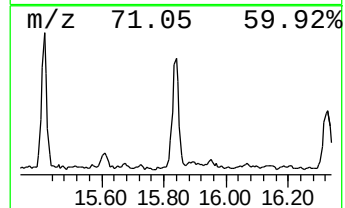
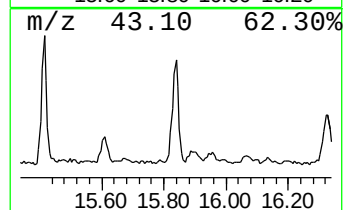
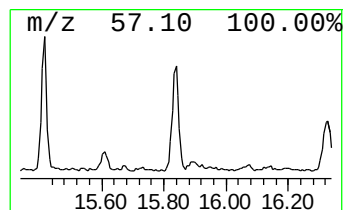
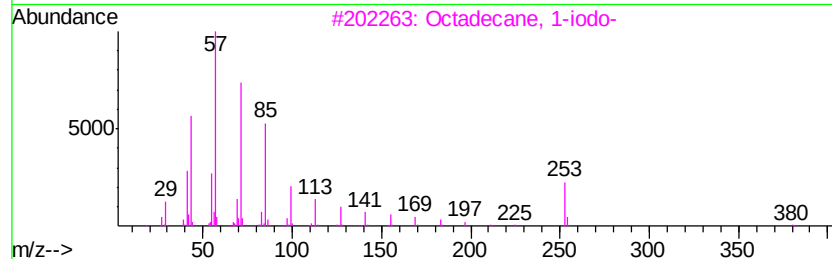
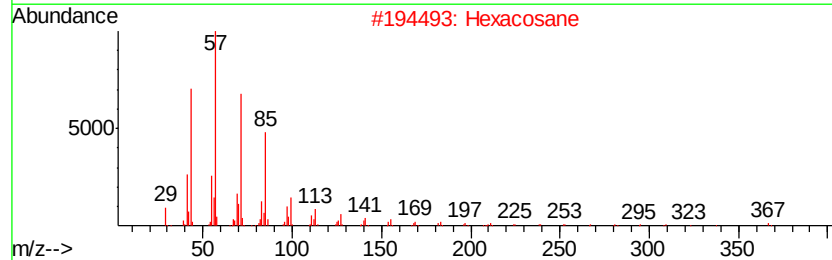
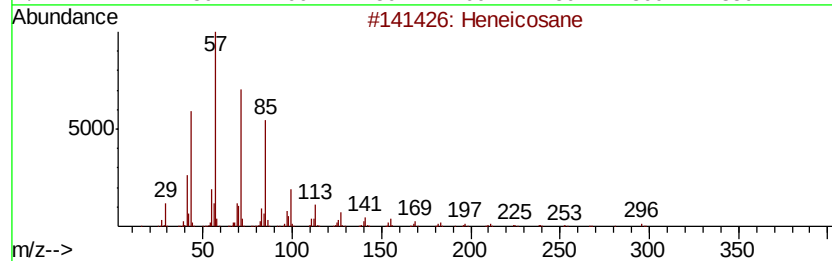
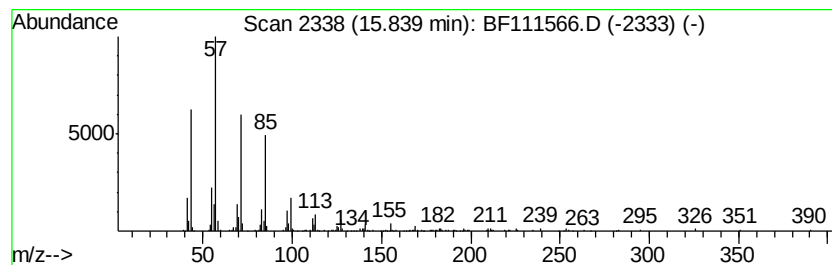
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Heneicosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.84	8.49 ng	321326	Perylene-d12	15.38

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heneicosane	296	C21H44	000629-94-7	91
2		Hexacosane	366	C26H54	000630-01-3	87
3		Octadecane, 1-iodo-	380	C18H37I	000629-93-6	87
4		Tetracosane	338	C24H50	000646-31-1	87
5		Heptadecane	240	C17H36	000629-78-7	86



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121718\
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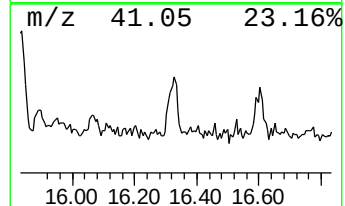
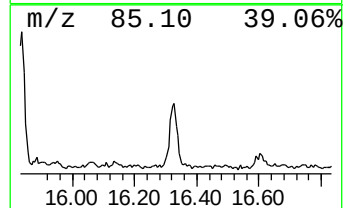
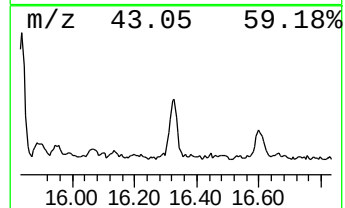
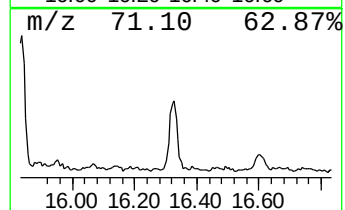
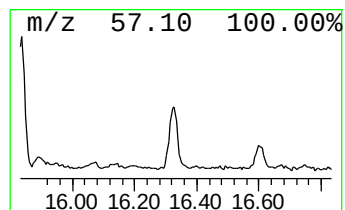
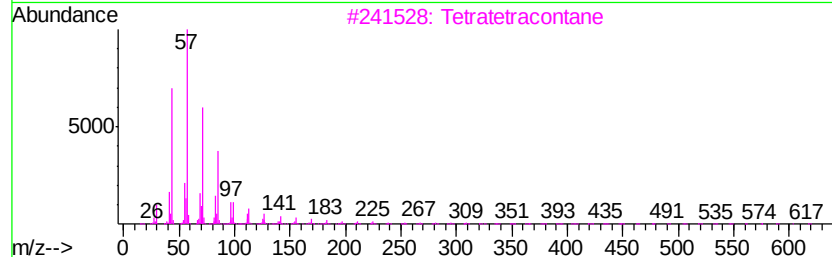
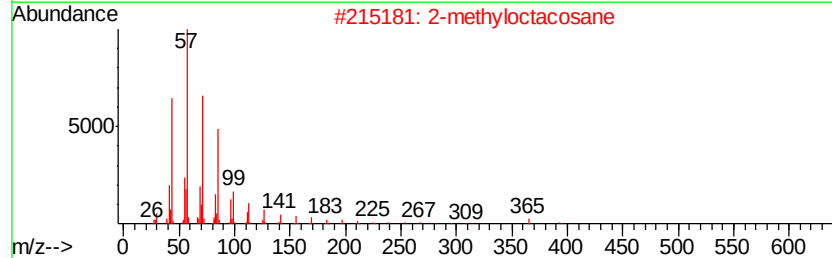
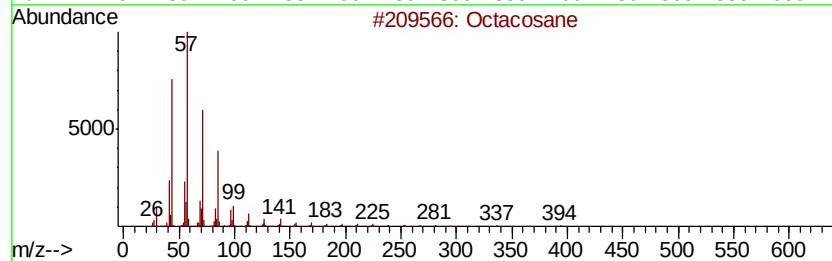
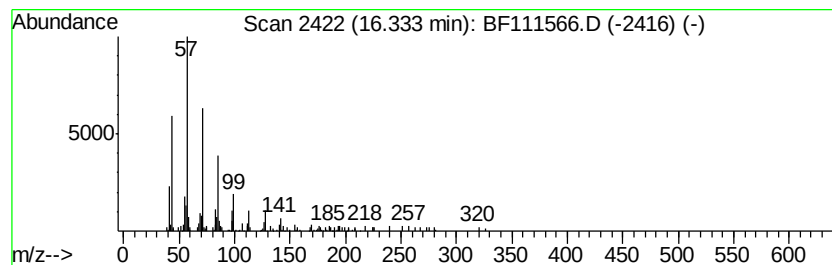
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 Octacosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.	
16.33	4.50 ng	170062	Perylene-d12	15.38	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	87
2	2-methyloctacosane	408	C29H60	1000376-72-8	86
3	Tetratetracontane	619	C44H90	007098-22-8	86
4	Triacontane	422	C30H62	000638-68-6	86
5	Pentacosane	352	C25H52	000629-99-2	86



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121718\
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Acq On : 18 Dec 2018 3:48
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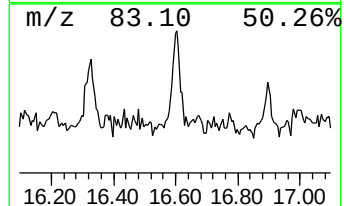
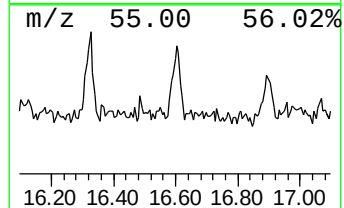
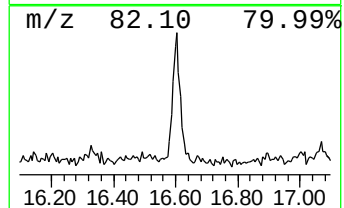
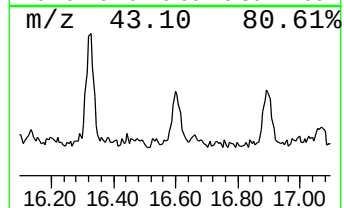
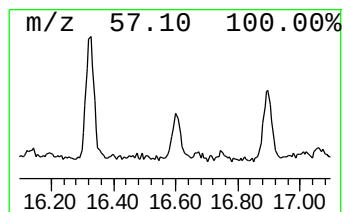
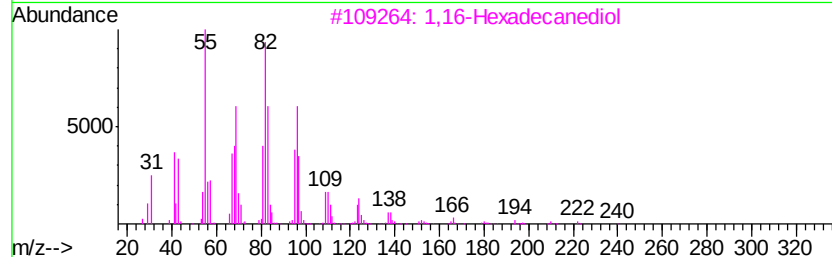
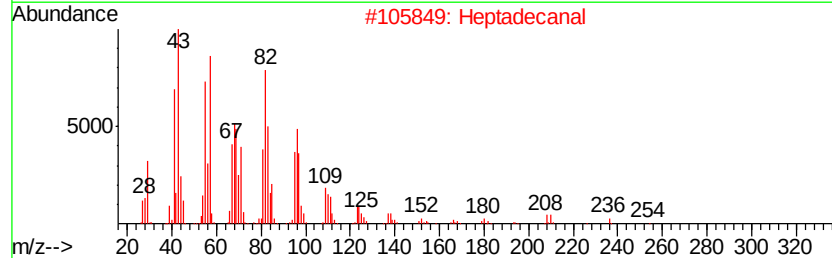
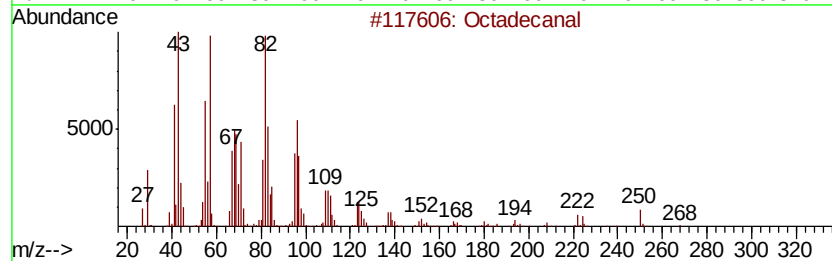
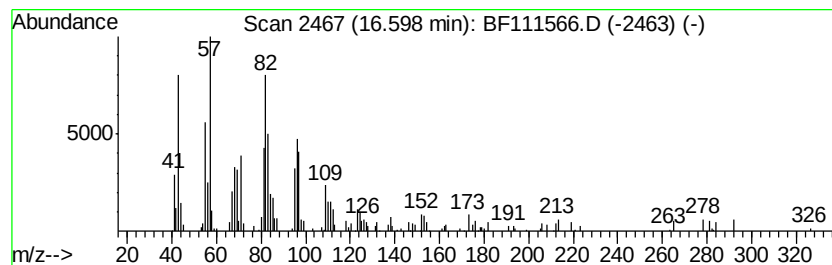
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 Octadecanal Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.60	3.72 ng	140571	Perylene-d12	15.38

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanal	268	C18H36O	000638-66-4	87
2			Heptadecanal	254	C17H34O	1000376-70-0	64
3			1,16-Hexadecanediol	258	C16H34O2	007735-42-4	58
4			16-Heptadecenal	252	C17H32O	1000144-57-9	58
5			Bicyclo[4.1.0]heptane, 7-butyl-	152	C11H20	018645-10-8	53



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121718\
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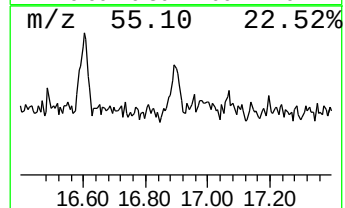
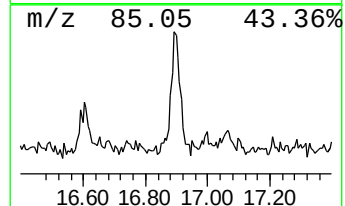
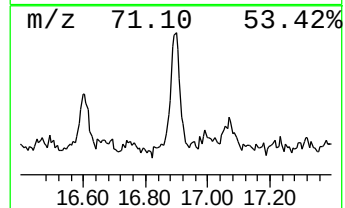
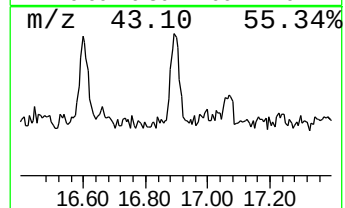
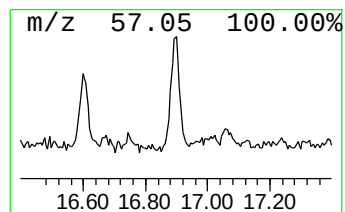
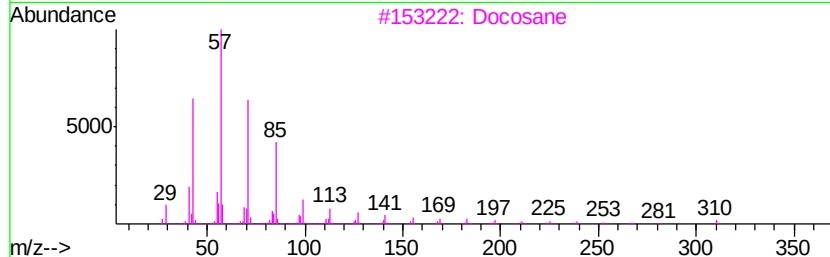
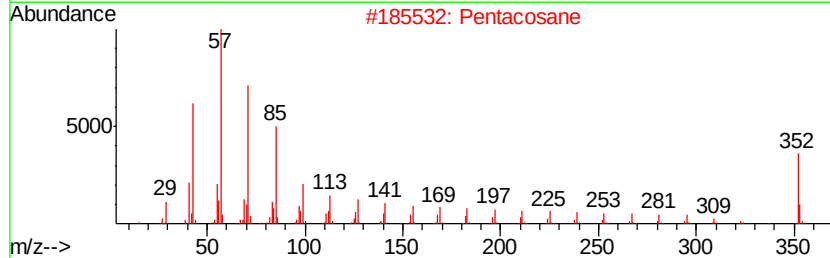
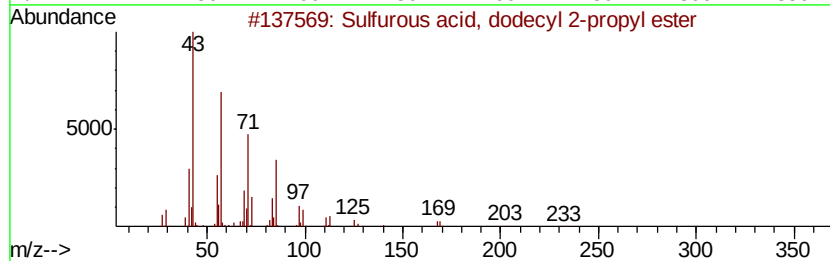
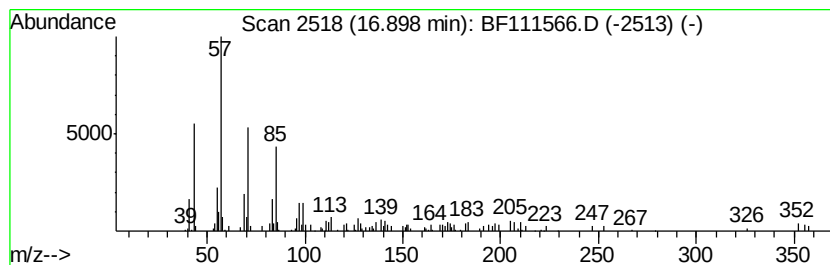
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 15 Sulfurous acid, dodecyl 2-p... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.90	3.16 ng	119625	Perylene-d12	15.38

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Sulfurous acid, dodecyl 2-propyl...	292	C15H32O3S	1000309-12-3	80
2		Pentacosane	352	C25H52	000629-99-2	72
3		Docosane	310	C22H46	000629-97-0	64
4		Hexacosane	366	C26H54	000630-01-3	64
5		Pentadecane, 8-hexyl-	296	C21H44	013475-75-7	64



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ALS Vial : 27 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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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
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unknown6.56	6.56	56.4 ng		2863680	1	6.79	1014730	20.0
n-Hexadecanoic acid	11.84	5.7 ng		273086	4	11.31	953237	20.0
Heptadecyl heptaf...	13.79	7.0 ng		383443	5	13.94	1089860	20.0
Pentacosane	14.12	2.3 ng		124938	5	13.94	1089860	20.0
Octadecane	14.42	6.1 ng		331639	5	13.94	1089860	20.0
Squalene	14.79	3.0 ng		112449	6	15.38	756514	20.0
Heneicosane	15.84	8.5 ng		321326	6	15.38	756514	20.0
Octacosane	16.33	4.5 ng		170062	6	15.38	756514	20.0
Octadecanal	16.60	3.7 ng		140571	6	15.38	756514	20.0
Sulfurous acid, d...	16.90	3.2 ng		119625	6	15.38	756514	20.0