

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091418\
 Data File : BF108998.D
 Acq On : 14 Sep 2018 16:49
 Operator : JU/SJ
 Sample : J4906-01
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SP-PIT-3

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-BF091418.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	4.913	434	438	450	rVB	83941	108726	3.84%	0.384%
2	5.331	503	509	512	rBV	2220352	2356994	83.31%	8.316%
3	6.354	677	683	687	rBV	2575850	2558242	90.42%	9.026%
4	6.489	701	706	709	rBV	2715964	2506690	88.60%	8.844%
5	6.719	741	745	748	rBV	1164117	877785	31.03%	3.097%
6	6.878	768	772	775	rBV	2234561	1877156	66.35%	6.623%
7	7.278	835	840	843	rBV	1833165	1603905	56.69%	5.659%
8	8.001	959	963	966	rBV	1422683	1143838	40.43%	4.036%
9	9.077	1141	1146	1149	rBV	3279379	2728075	96.43%	9.626%
10	9.466	1209	1212	1215	rBV	312957	257290	9.09%	0.908%
11	9.748	1256	1260	1264	rBV2	1492217	1333631	47.14%	4.705%
12	10.530	1389	1393	1406	rBV	2053486	1924092	68.01%	6.789%
13	11.224	1507	1511	1514	rBV	1645796	1405640	49.68%	4.960%
14	11.766	1599	1603	1607	rBV	166133	146027	5.16%	0.515%
15	12.430	1713	1716	1719	rBV	50999	42319	1.50%	0.149%
16	12.654	1748	1754	1757	rBV2	45261	59606	2.11%	0.210%
17	12.813	1776	1781	1784	rBV	2917441	2829207	100.00%	9.982%
18	13.054	1819	1822	1826	rVB	51522	48798	1.72%	0.172%
19	13.295	1854	1863	1869	rBV2	49498	75872	2.68%	0.268%
20	13.395	1878	1880	1883	rBV	64370	57453	2.03%	0.203%
21	13.718	1930	1935	1947	rBV2	237120	382005	13.50%	1.348%
22	13.854	1953	1958	1961	rBV	1327674	1277157	45.14%	4.506%
23	14.042	1986	1990	1993	rBV	110811	107984	3.82%	0.381%
24	14.342	2038	2041	2045	rBV	143265	129146	4.56%	0.456%
25	14.636	2088	2091	2096	rVB	145144	144137	5.09%	0.509%
26	14.707	2100	2103	2107	rVB	116552	106438	3.76%	0.376%
27	14.954	2141	2145	2150	rBV	166985	188129	6.65%	0.664%
28	15.254	2191	2196	2201	rBV	886150	1024525	36.21%	3.615%
29	15.312	2201	2206	2213	rVB	221764	281811	9.96%	0.994%
30	15.718	2269	2275	2280	rBV	221071	334793	11.83%	1.181%
31	16.183	2347	2354	2364	rVB	141853	263080	9.30%	0.928%
32	16.730	2441	2447	2453	rBV2	54634	107722	3.81%	0.380%
33	17.365	2551	2555	2564	rVB4	23979	53853	1.90%	0.190%

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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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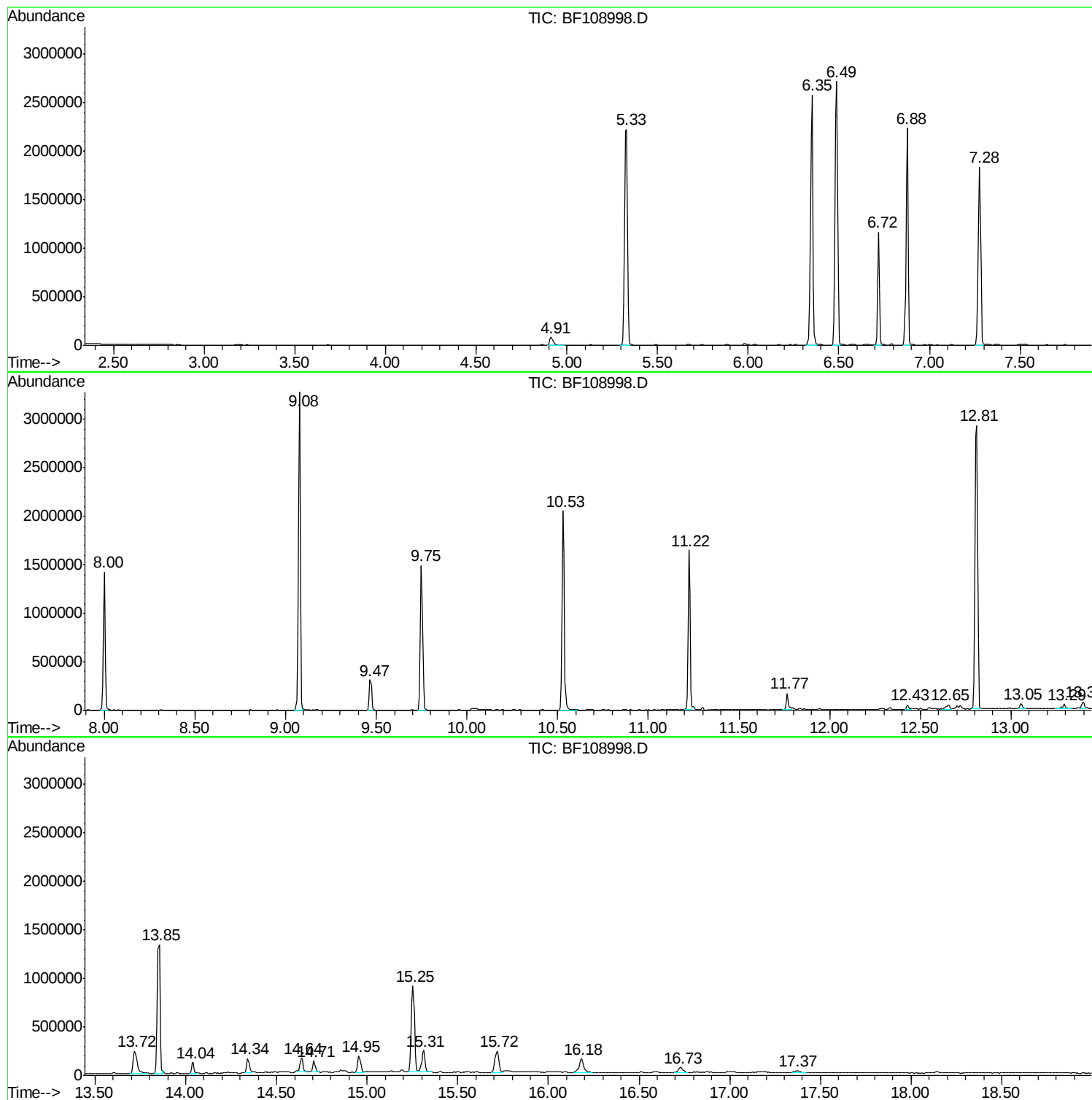
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF091418.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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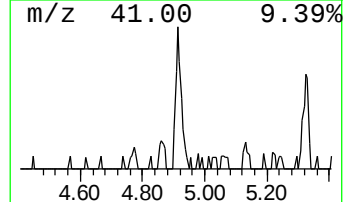
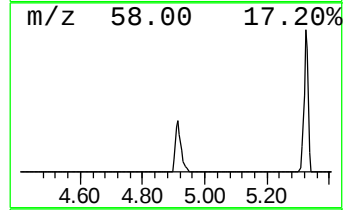
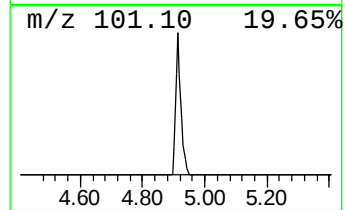
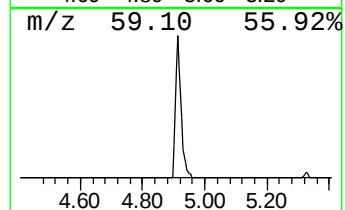
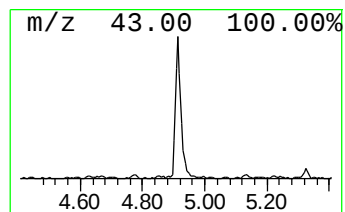
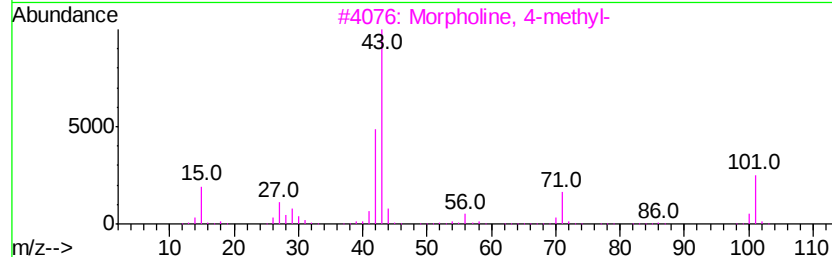
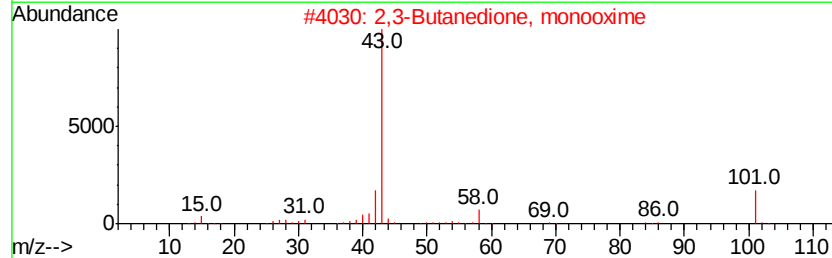
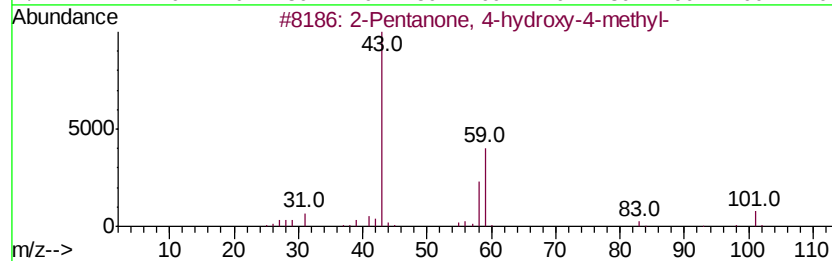
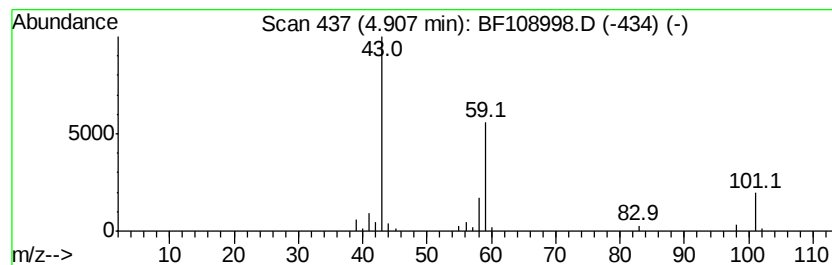
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.91	2.48 ng	108726	1,4-Dichlorobenzene-d4	6.72

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
3		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4		5-Hexen-2-one	98	C6H10O	000109-49-9	9
5		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9



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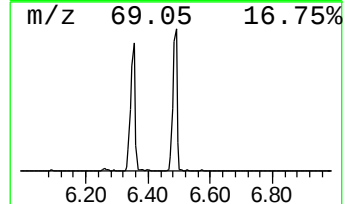
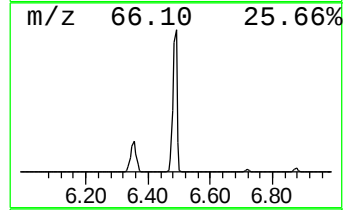
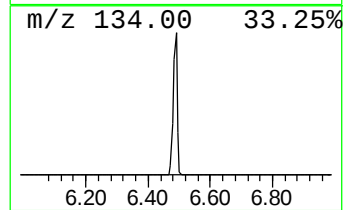
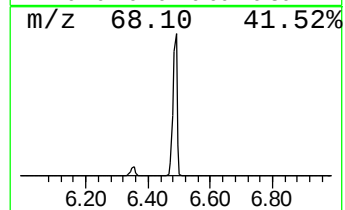
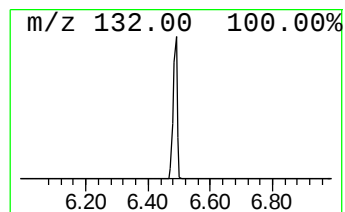
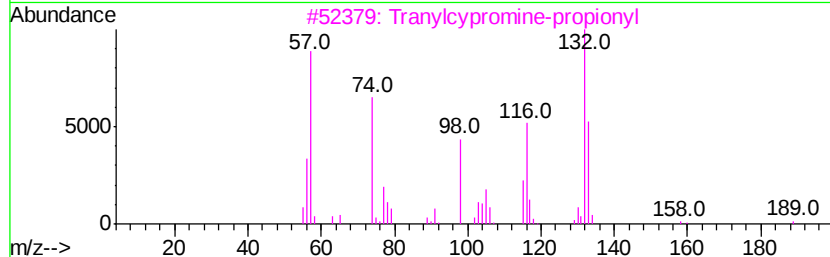
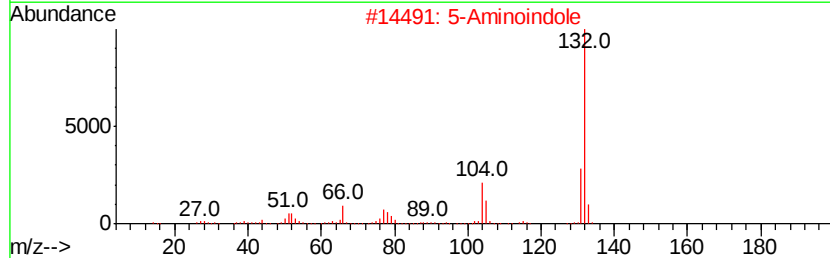
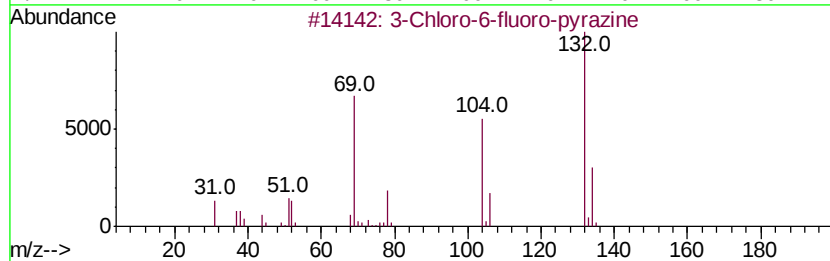
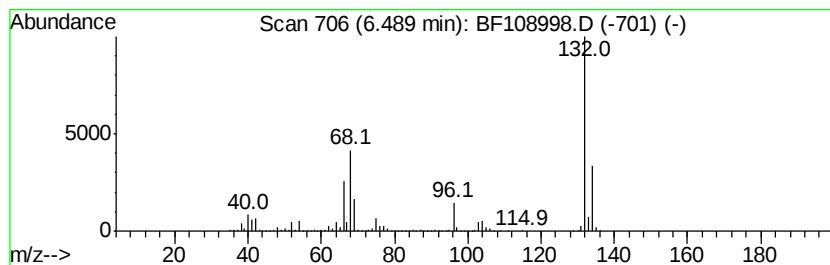
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.49 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.49	57.11 ng	2506690	1,4-Dichlorobenzene-d4	6.72

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2			5-Aminoindole	132	C8H8N2	005192-03-0	12
3			Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	10
4			Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5			4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9



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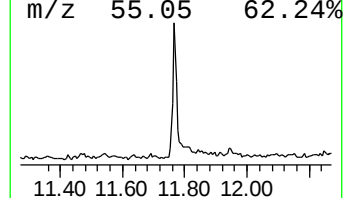
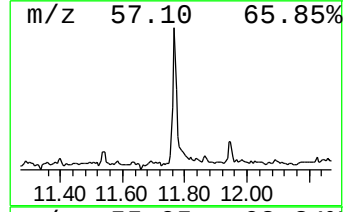
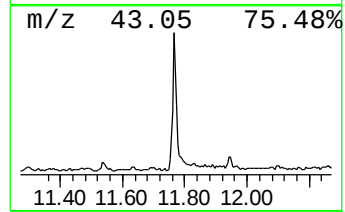
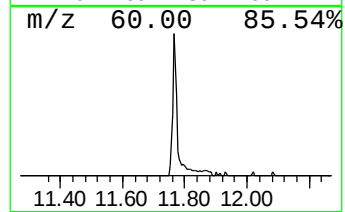
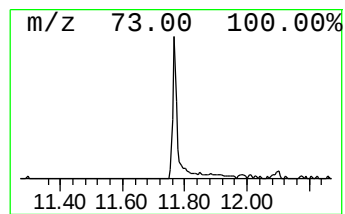
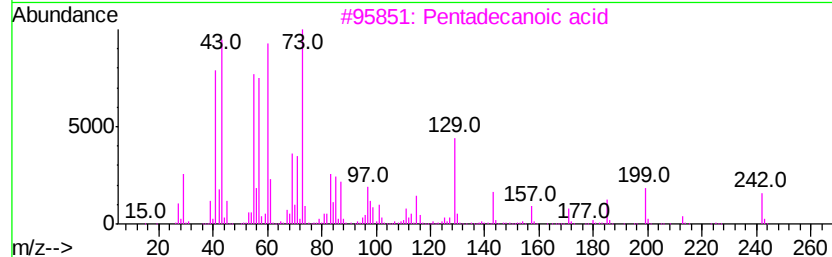
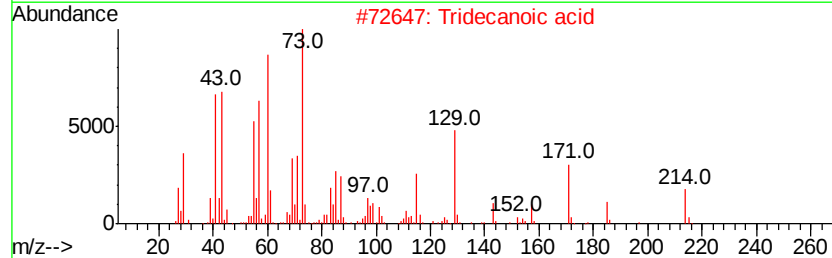
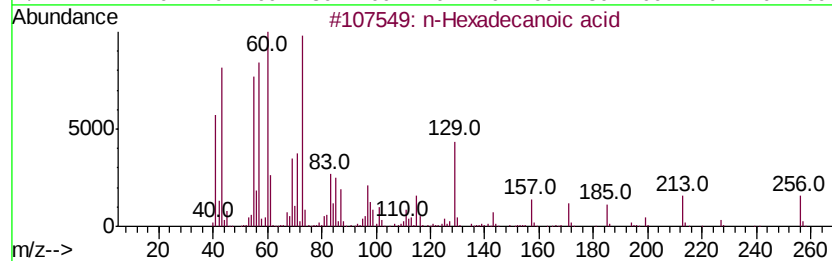
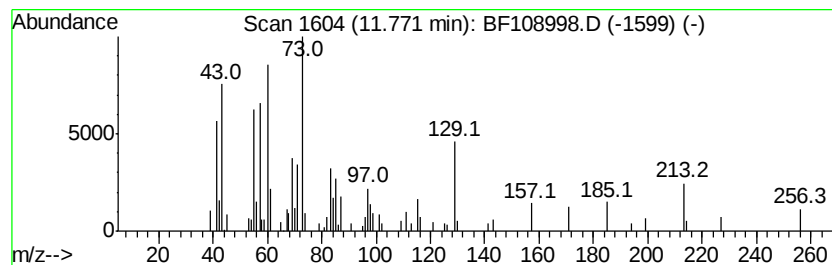
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.77	2.08 ng	146027	Phenanthrene-d10	11.22

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2		Tridecanoic acid	214	C13H26O2	000638-53-9	97
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	74
5		Dodecanoic acid	200	C12H24O2	000143-07-7	59



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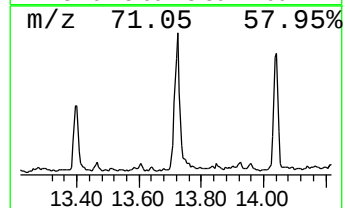
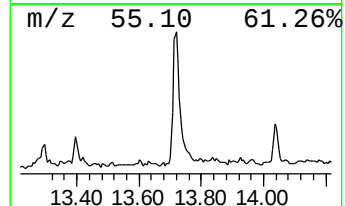
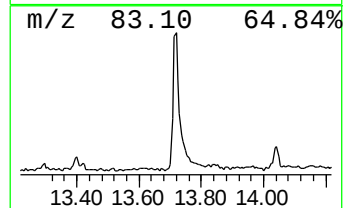
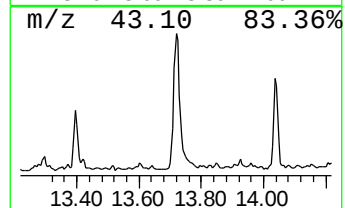
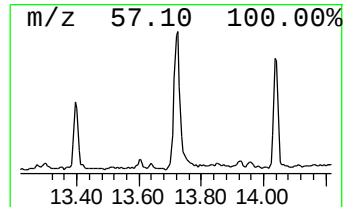
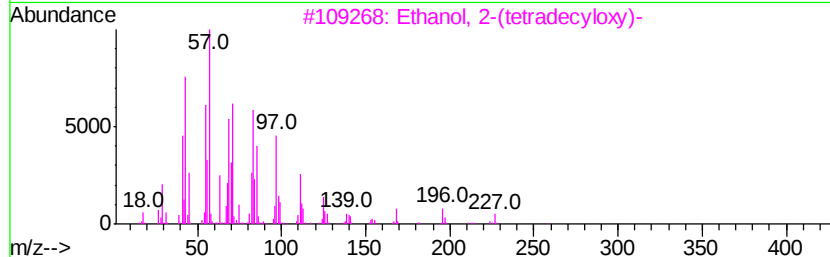
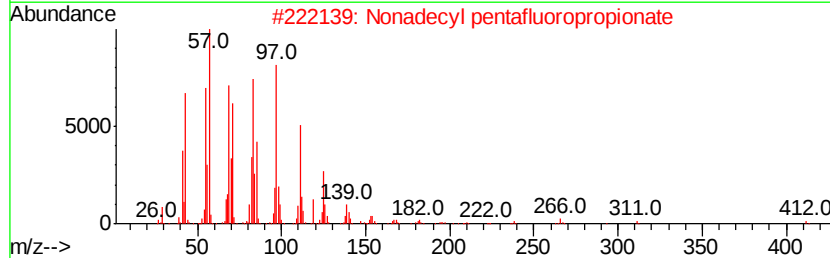
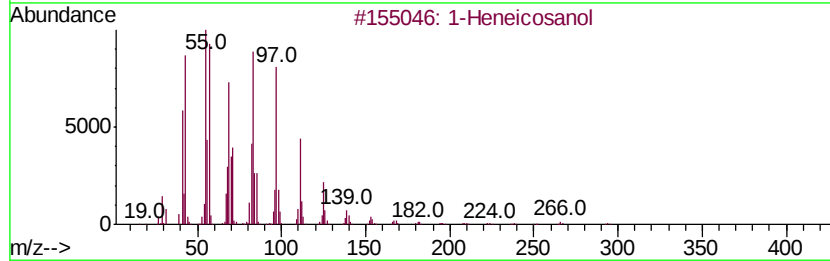
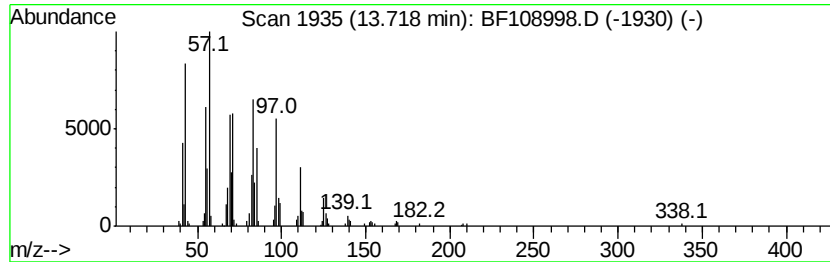
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 1-Heneicosanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.72	5.98 ng	382005	Chrysene-d12	13.85

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Heneicosanol	312	C21H44O	015594-90-8	93
2		Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	91
3		Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	90
4		Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	81
5		Pentafluoropropionic acid, octad...	416	C21H37F5O2	959261-25-7	81



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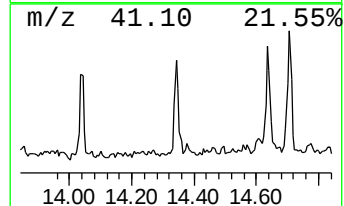
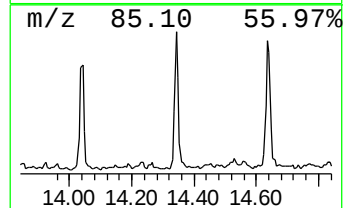
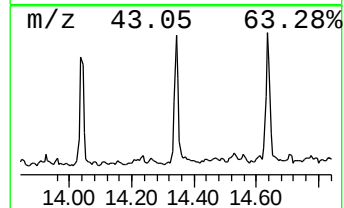
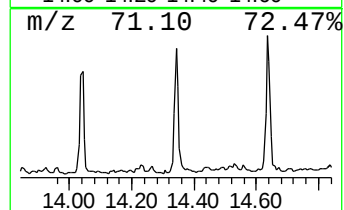
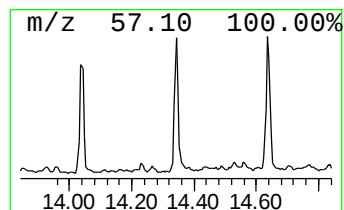
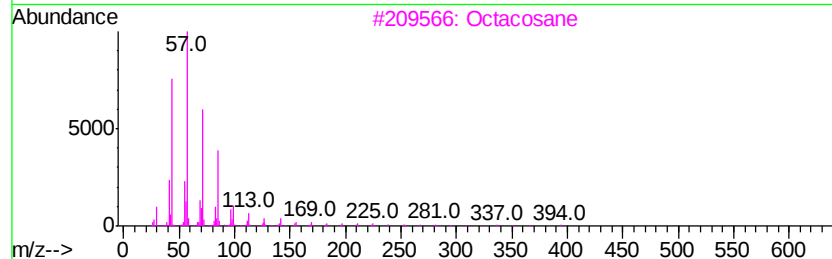
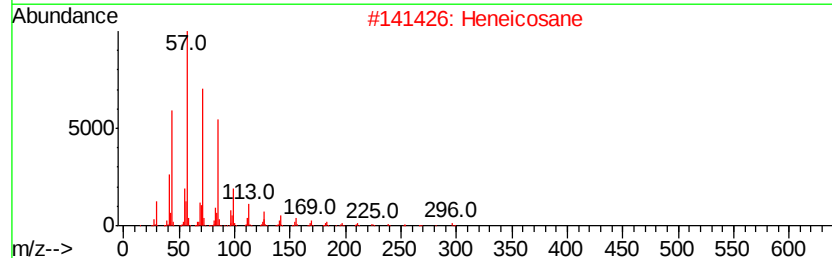
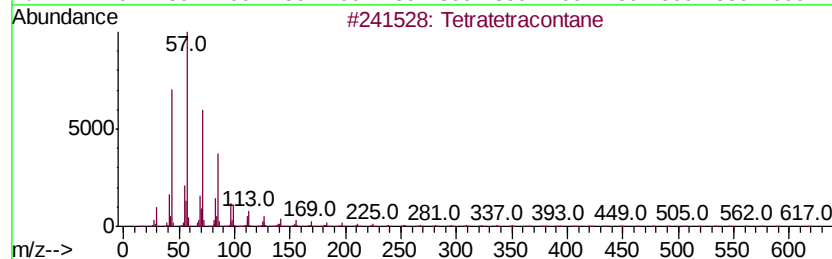
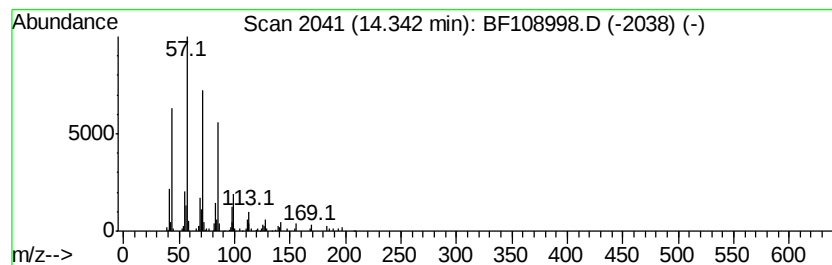
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Peak Number 6 Tetratetracontane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.34	2.02 ng	129146	Chrysene-d12	13.85

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tetratetracontane	619	C44H90	007098-22-8	91
2		Heneicosane	296	C21H44	000629-94-7	91
3		Octacosane	394	C28H58	000630-02-4	91
4		Hexacosane	366	C26H54	000630-01-3	91
5		Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091418\
Data File : BF108998.D
Acq On : 14 Sep 2018 16:49
Operator : JU/SJ
Sample : J4906-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
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ClientSampleId :
SP-PIT-3

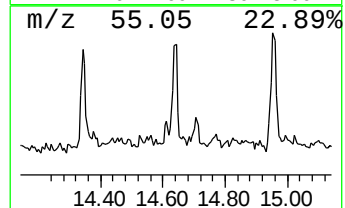
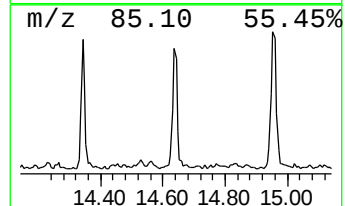
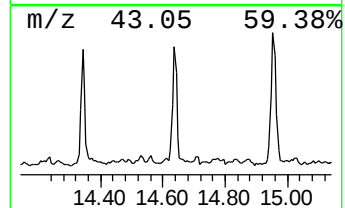
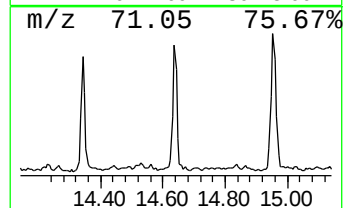
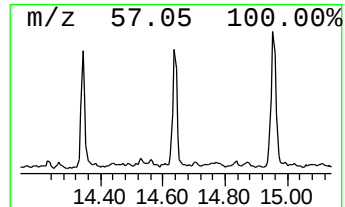
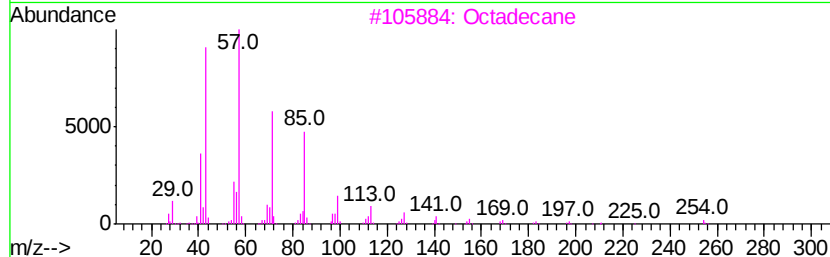
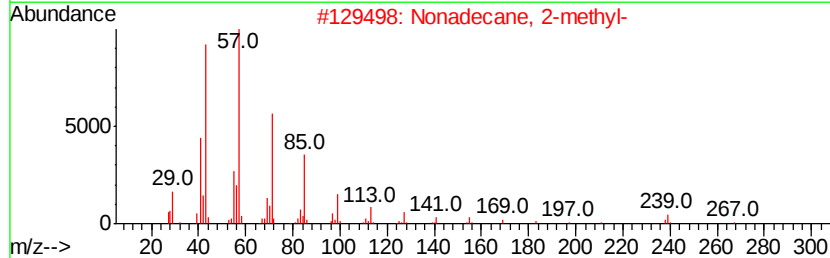
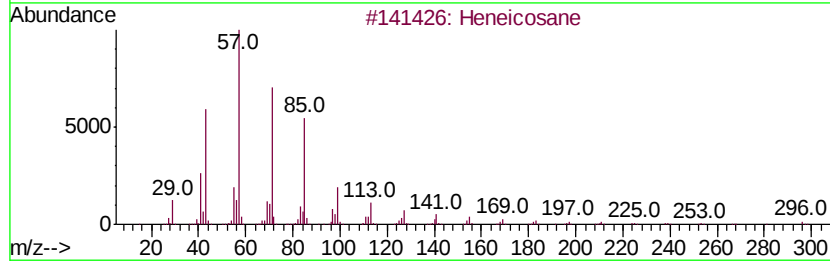
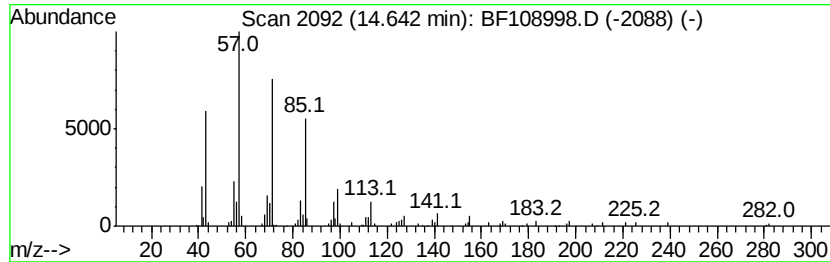
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Heneicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.64	2.81 ng	144137	Perylene-d12	15.25

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heneicosane	296	C21H44	000629-94-7	91
2		Nonadecane, 2-methyl-	282	C20H42	001560-86-7	91
3		Octadecane	254	C18H38	000593-45-3	90
4		Hexadecane, 1-iodo-	352	C16H33I	000544-77-4	90
5		Tetracosane	338	C24H50	000646-31-1	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091418\
Data File : BF108998.D
Acq On : 14 Sep 2018 16:49
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ClientSampleId :
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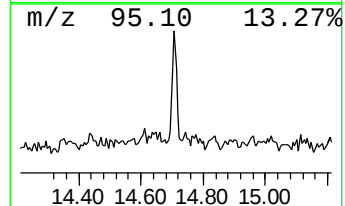
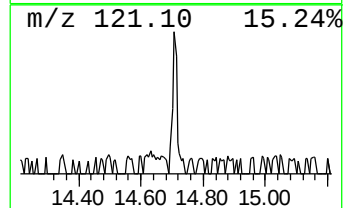
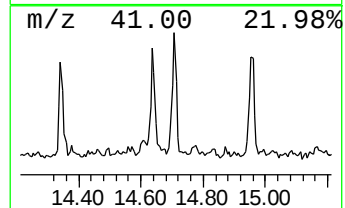
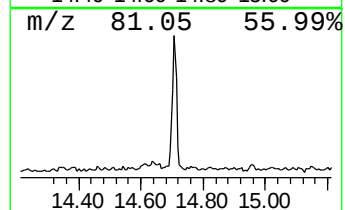
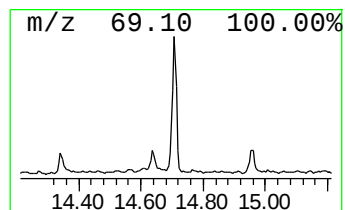
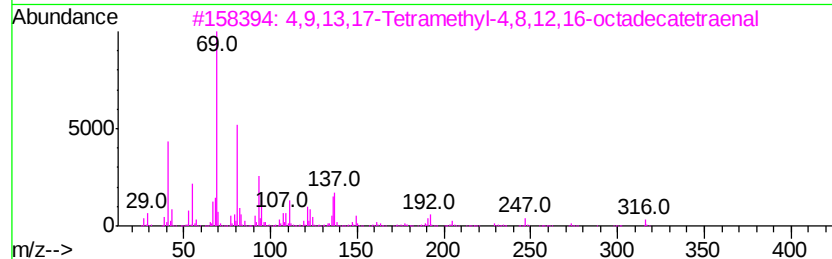
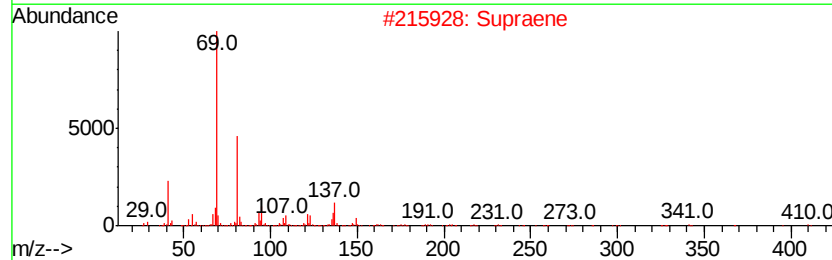
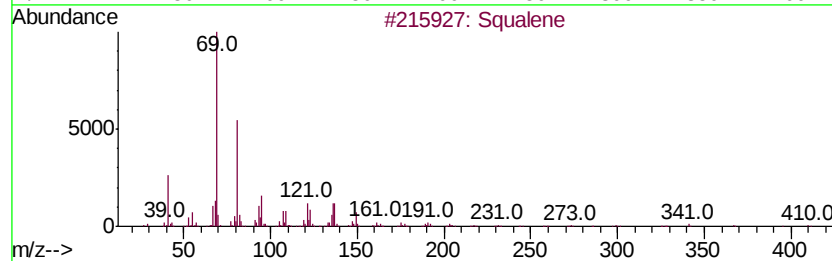
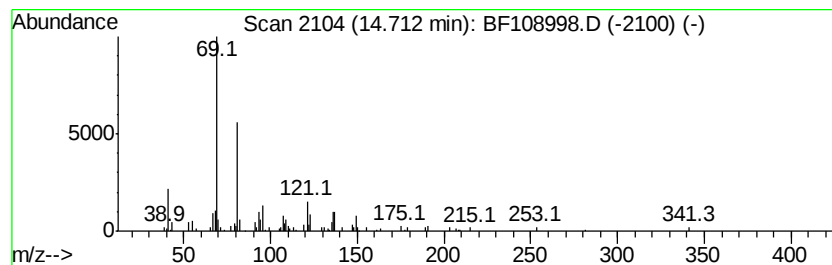
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Squalene Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.71	2.08 ng	106438	Perylene-d12	15.25

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Squalene	410	C30H50	000111-02-4	91
2		Supraene	410	C30H50	007683-64-9	87
3		4,9,13,17-Tetramethyl-4,8,12,16-...	316	C22H36O	056882-09-8	83
4		1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	80
5		2,6,10,14-Hexadecatetraenoic aci...	332	C22H36O2	024035-35-6	72



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091418\
Data File : BF108998.D
Acq On : 14 Sep 2018 16:49
Operator : JU/SJ
Sample : J4906-01
Misc :
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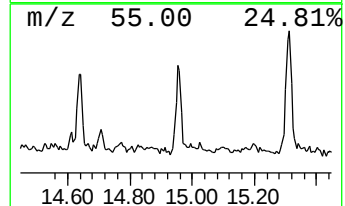
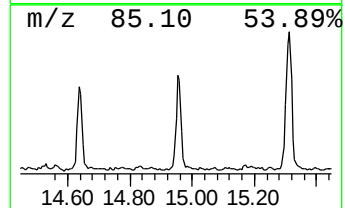
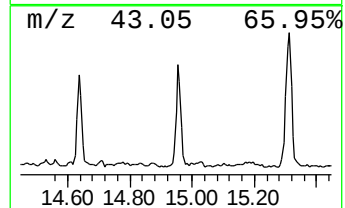
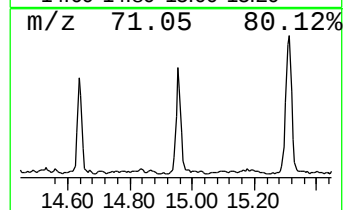
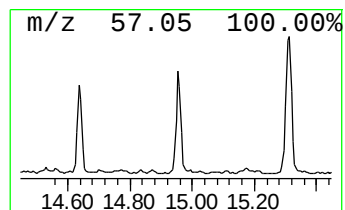
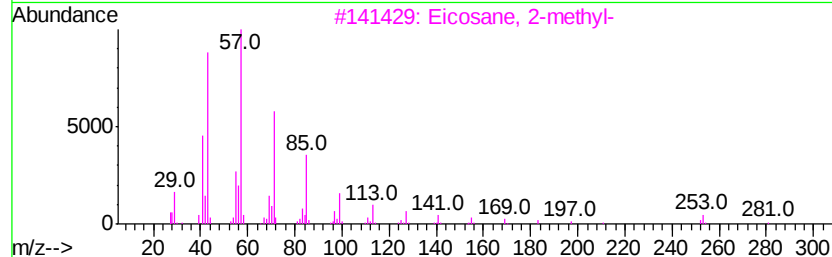
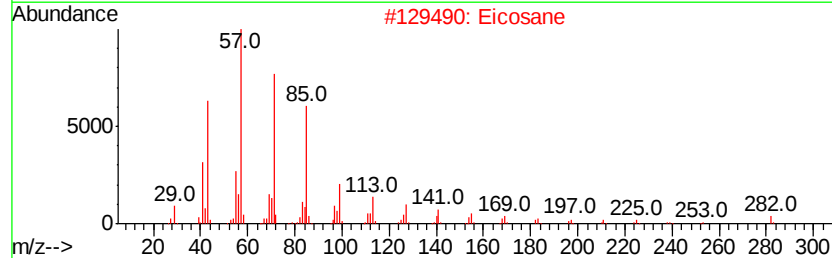
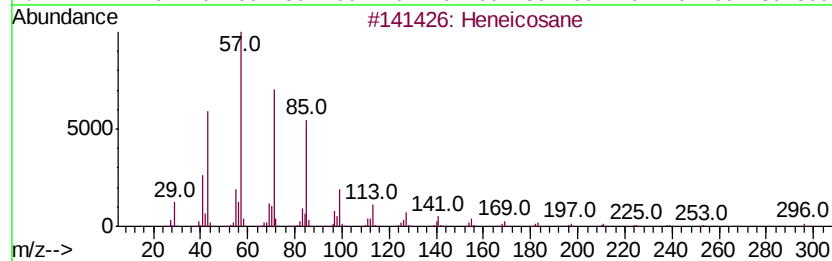
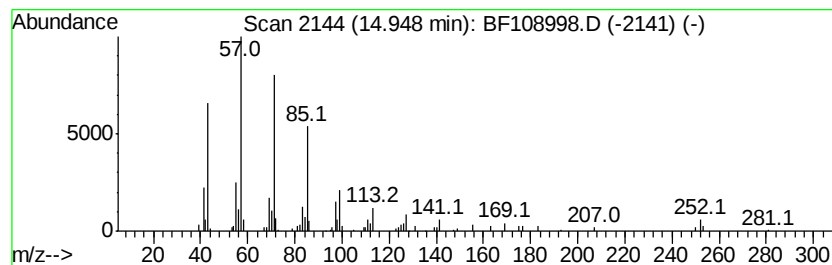
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Eicosane, 2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.95	3.67 ng	188129	Perylene-d12	15.25

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heneicosane	296	C21H44	000629-94-7	91
2		Eicosane	282	C20H42	000112-95-8	91
3		Eicosane, 2-methyl-	296	C21H44	001560-84-5	91
4		Tetracosane	338	C24H50	000646-31-1	91
5		triacontane	422	C30H62	000638-68-6	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091418\
Data File : BF108998.D
Acq On : 14 Sep 2018 16:49
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Misc :
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ClientSampleId :
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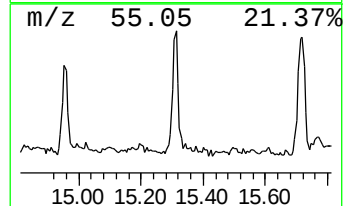
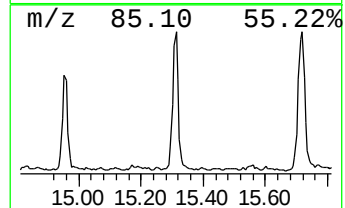
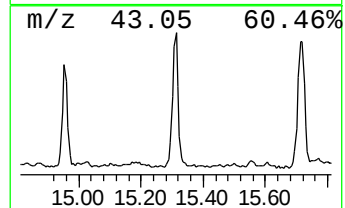
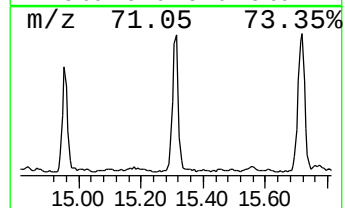
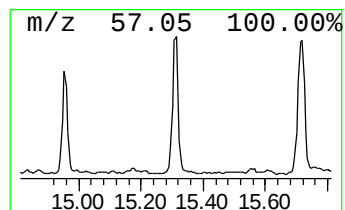
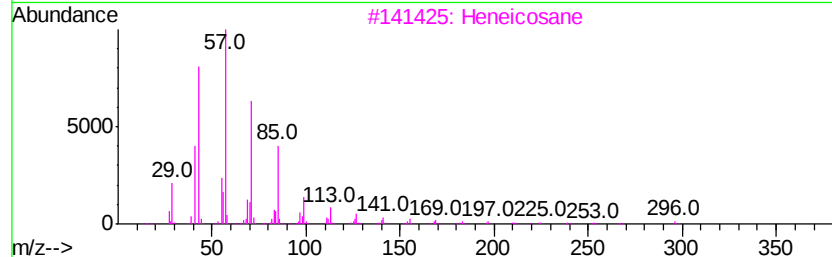
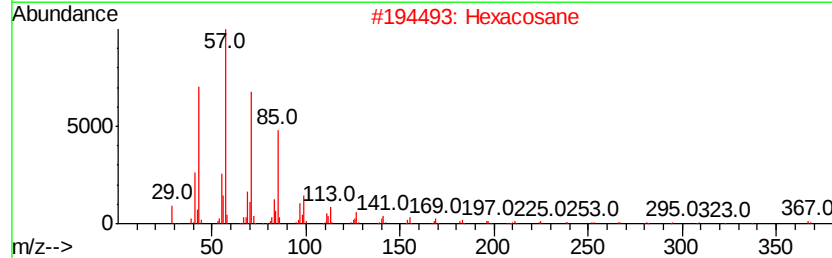
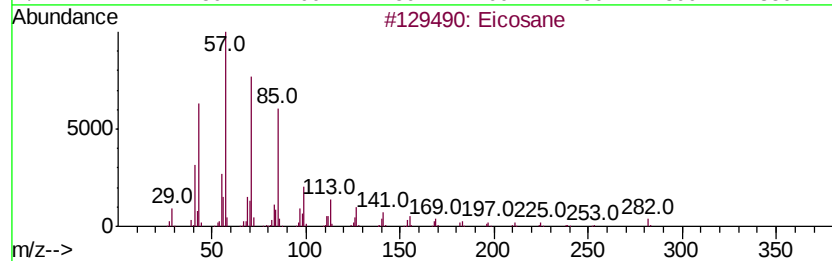
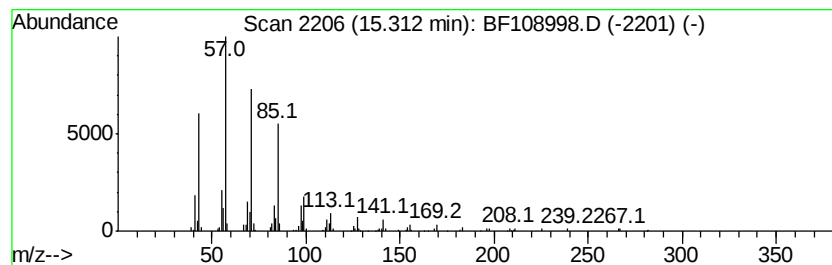
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Eicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.31	5.50 ng	281811	Perylene-d12	15.25

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Eicosane	282	C20H42	000112-95-8	95
2		Hexacosane	366	C26H54	000630-01-3	91
3		Heneicosane	296	C21H44	000629-94-7	91
4		Octadecane	254	C18H38	000593-45-3	87
5		Heptadecane	240	C17H36	000629-78-7	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091418\
Data File : BF108998.D
Acq On : 14 Sep 2018 16:49
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Misc :
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ClientSampleId :
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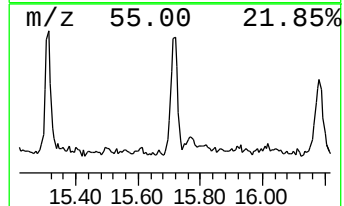
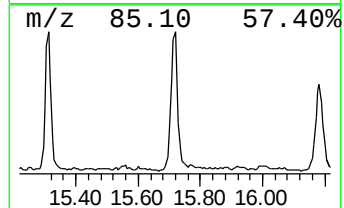
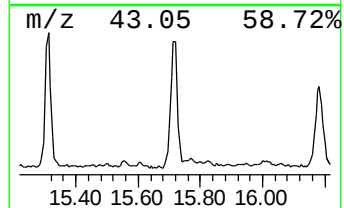
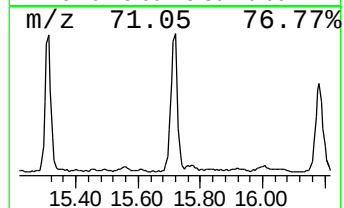
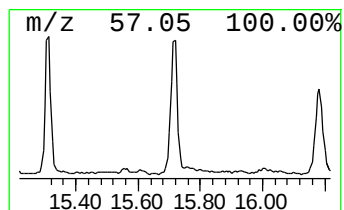
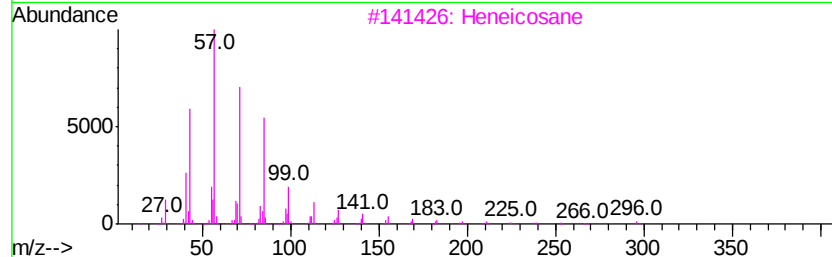
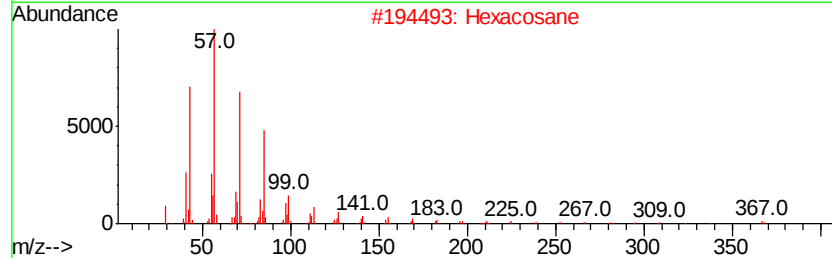
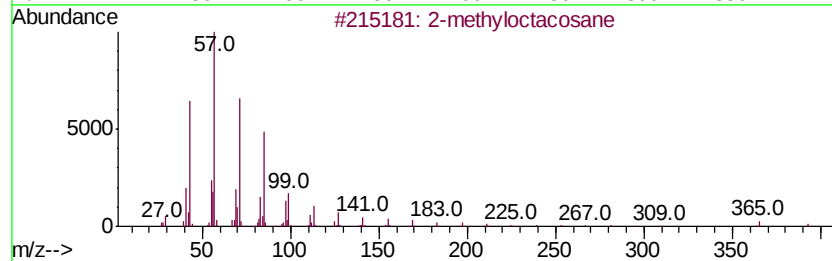
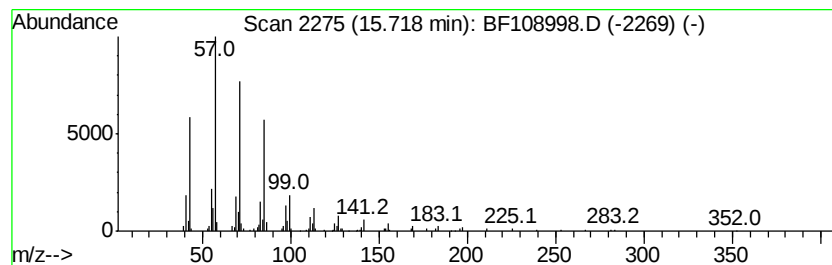
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 2-methyloctacosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.72	6.54 ng	334793	Perylene-d12	15.25

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-methyloctacosane	408	C29H60	1000376-72-8	91
2			Hexacosane	366	C26H54	000630-01-3	91
3			Heneicosane	296	C21H44	000629-94-7	91
4			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
5			Pentadecane, 8-hexyl-	296	C21H44	013475-75-7	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091418\
Data File : BF108998.D
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ClientSampleId :
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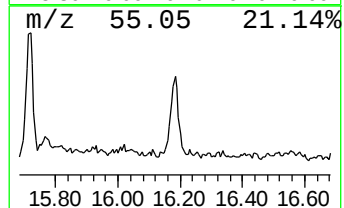
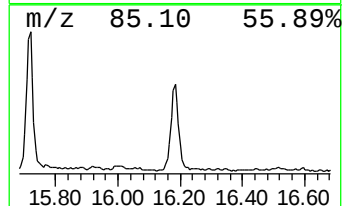
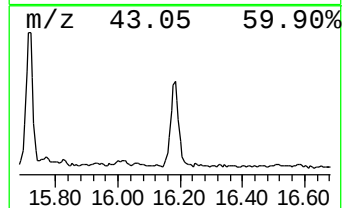
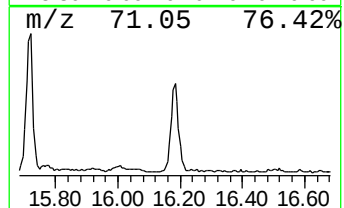
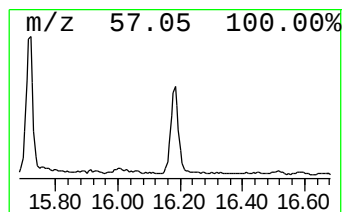
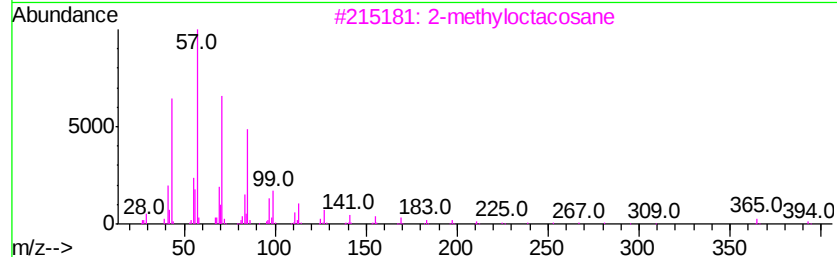
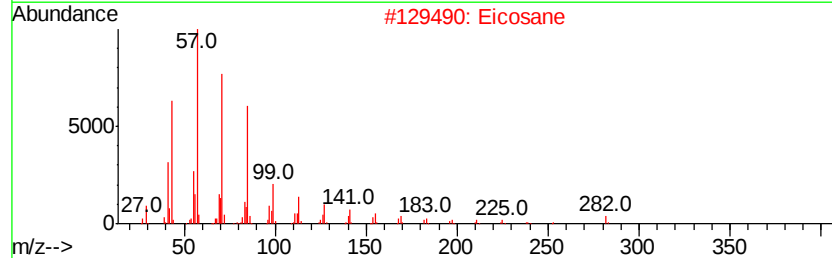
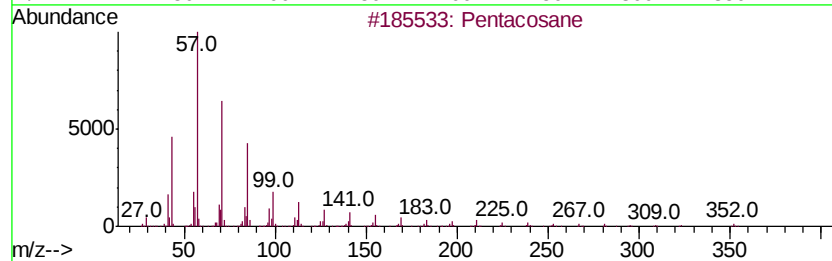
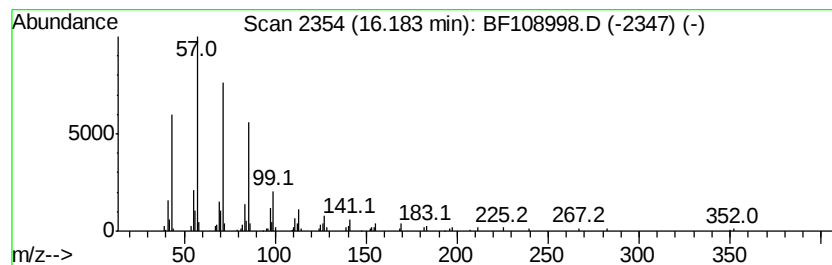
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Pentacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.18	5.14 ng	263080	Perylene-d12	15.25

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentacosane	352	C25H52	000629-99-2	96
2		Eicosane	282	C20H42	000112-95-8	94
3		2-methyloctacosane	408	C29H60	1000376-72-8	91
4		Tetracosane	338	C24H50	000646-31-1	91
5		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091418\
Data File : BF108998.D
Acq On : 14 Sep 2018 16:49
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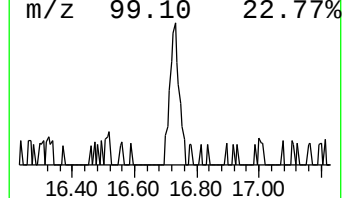
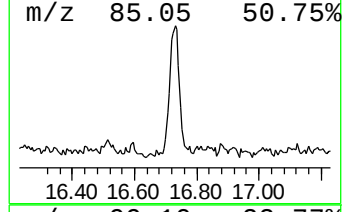
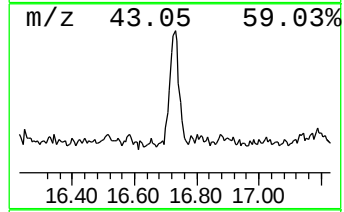
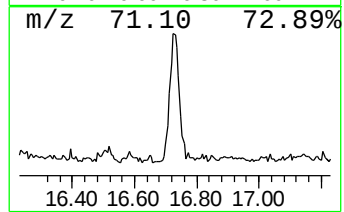
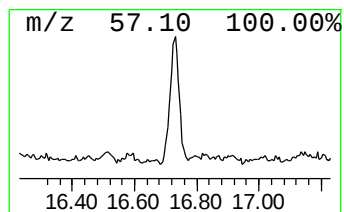
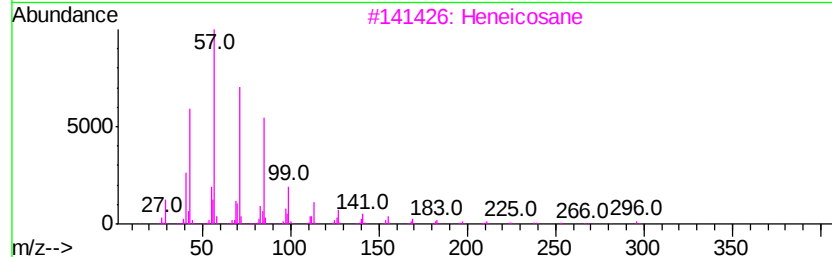
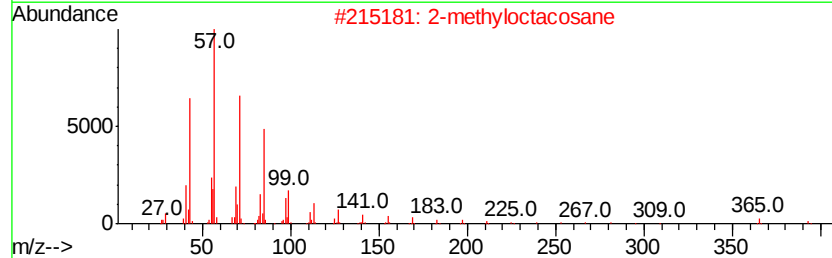
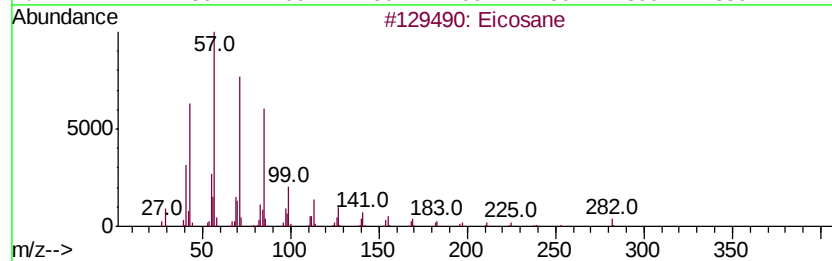
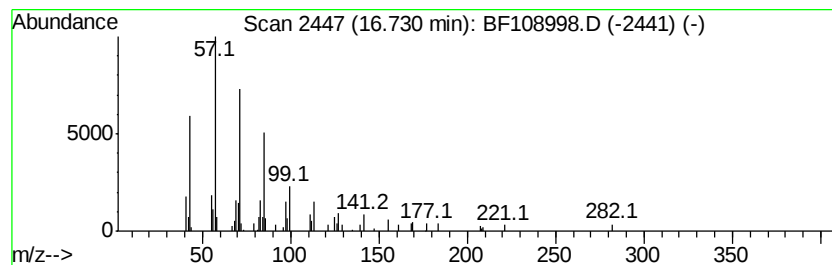
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 Hentriacontane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.73	2.10 ng	107722	Perylene-d12	15.25

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Eicosane	282	C20H42	000112-95-8	98
2		2-methyloctacosane	408	C29H60	1000376-72-8	91
3		Heneicosane	296	C21H44	000629-94-7	90
4		Hentriacontane	437	C31H64	000630-04-6	90
5		Octacosane	394	C28H58	000630-02-4	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF091418\
Data File : BF108998.D
Acq On : 14 Sep 2018 16:49
Operator : JU/SJ
Sample : J4906-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-PIT-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091418.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...	4.91	2.5	ng	108726	1	6.72	877785	20.0
unknown6.49	6.49	57.1	ng	2506690	1	6.72	877785	20.0
n-Hexadecanoic acid	11.77	2.1	ng	146027	4	11.22	1405640	20.0
1-Heneicosanol	13.72	6.0	ng	382005	5	13.85	1277160	20.0
Tetratetracontane	14.34	2.0	ng	129146	5	13.85	1277160	20.0
Heneicosane	14.64	2.8	ng	144137	6	15.25	1024530	20.0
Squalene	14.71	2.1	ng	106438	6	15.25	1024530	20.0
Eicosane, 2-methyl-	14.95	3.7	ng	188129	6	15.25	1024530	20.0
Eicosane	15.31	5.5	ng	281811	6	15.25	1024530	20.0
2-methyloctacosane	15.72	6.5	ng	334793	6	15.25	1024530	20.0
Pentacosane	16.18	5.1	ng	263080	6	15.25	1024530	20.0
Hentriacontane	16.73	2.1	ng	107722	6	15.25	1024530	20.0