

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF090518\
 Data File : BF108821.D
 Acq On : 6 Sep 2018 12:58
 Operator : JU/SJ
 Sample : J4724-14
 Misc :
 ALS Vial : 39 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 EP1-SUT-8USTS-W

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-BF090518.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	4.937	437	442	452	rBV	156572	213002	3.94%	0.430%
2	5.348	507	512	515	rBV	4822505	4928612	91.10%	9.947%
3	6.372	680	686	689	rBV	4993469	5175447	95.67%	10.445%
4	6.507	704	709	712	rBV	5332672	5103015	94.33%	10.299%
5	6.737	743	748	751	rBV	2161162	1708540	31.58%	3.448%
6	6.766	751	753	756	rVB	201099	168716	3.12%	0.340%
7	6.807	756	760	763	rBV2	67799	71362	1.32%	0.144%
8	6.895	768	775	778	rBV	4693845	4076733	75.36%	8.228%
9	7.031	792	798	801	rBV2	104805	122288	2.26%	0.247%
10	7.095	806	809	812	rBV	75073	79032	1.46%	0.159%
11	7.295	834	843	846	rBV	3575347	3269089	60.43%	6.598%
12	7.389	855	859	864	rVB5	52036	68141	1.26%	0.138%
13	7.466	864	872	876	rVB2	72330	121050	2.24%	0.244%
14	7.537	881	884	886	rBV2	90838	89370	1.65%	0.180%
15	7.678	904	908	910	rVB2	55840	69729	1.29%	0.141%
16	7.719	910	915	918	rBV3	55077	91037	1.68%	0.184%
17	7.784	923	926	929	rBV	76080	75091	1.39%	0.152%
18	8.019	961	966	969	rBV	2459298	2093894	38.70%	4.226%
19	8.095	977	979	985	rVB2	90230	93650	1.73%	0.189%
20	9.095	1144	1149	1152	rBV	6234455	5409963	100.00%	10.918%
21	9.219	1167	1170	1178	rVB2	48897	61730	1.14%	0.125%
22	9.483	1211	1215	1218	rBV	1655204	1307478	24.17%	2.639%
23	9.513	1218	1220	1226	rVB2	86504	80977	1.50%	0.163%
24	9.766	1259	1263	1267	rVB2	2477735	2107494	38.96%	4.253%
25	10.548	1392	1396	1399	rBV	3076965	2596541	48.00%	5.240%
26	11.242	1510	1514	1517	rBV	2131711	1693572	31.30%	3.418%
27	11.783	1603	1606	1615	rBV2	261879	303622	5.61%	0.613%
28	12.824	1779	1783	1787	rBV	4049164	3630478	67.11%	7.327%
29	13.101	1828	1830	1832	rBV	82574	64295	1.19%	0.130%
30	13.730	1934	1937	1944	rBV	557866	593221	10.97%	1.197%
31	13.866	1957	1960	1964	rVB	2168074	1951481	36.07%	3.938%
32	14.724	2104	2106	2110	rVB	298349	303136	5.60%	0.612%
33	15.271	2195	2199	2203	rVB	1108975	1307423	24.17%	2.639%
34	15.742	2276	2279	2283	rVB	131811	154598	2.86%	0.312%

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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	16.112	2339	2342	2350	rVB7	108233	184187	3.40%	0.372%
36	16.212	2355	2359	2364	rBV2	111757	182031	3.36%	0.367%

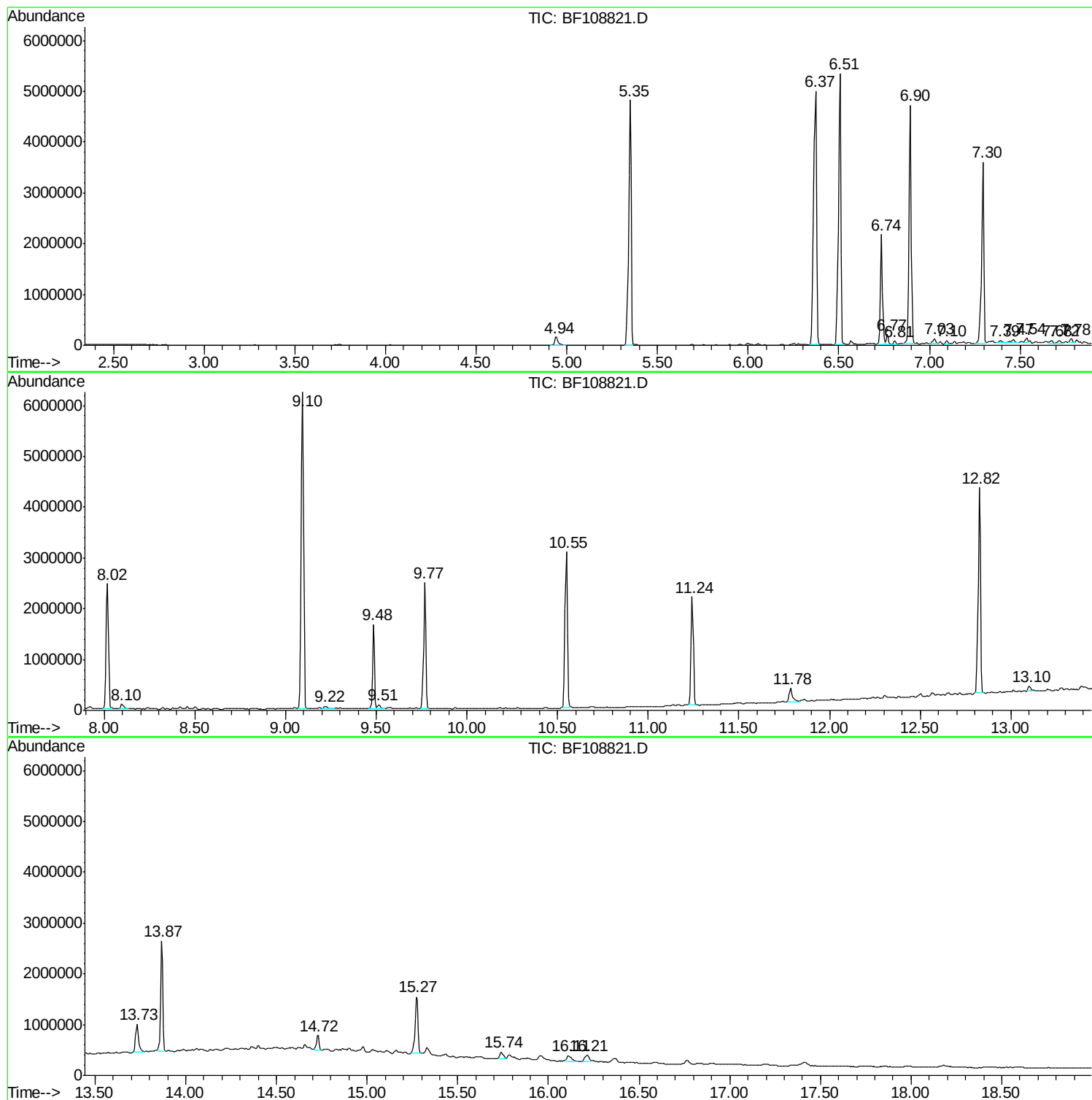
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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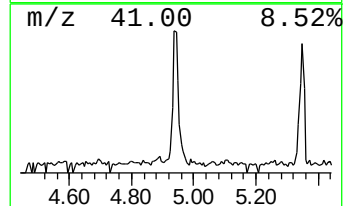
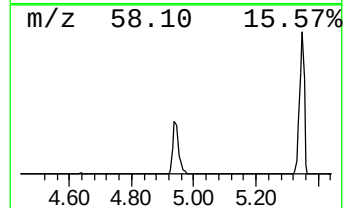
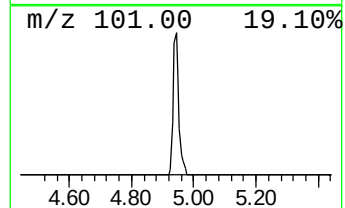
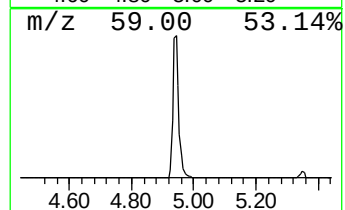
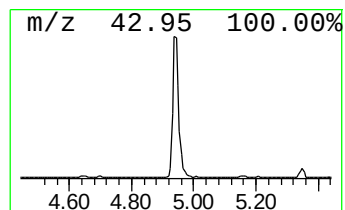
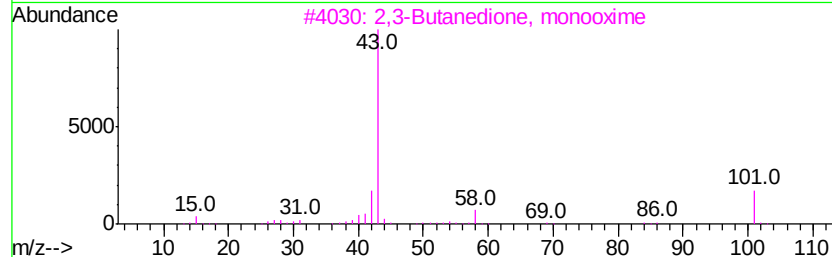
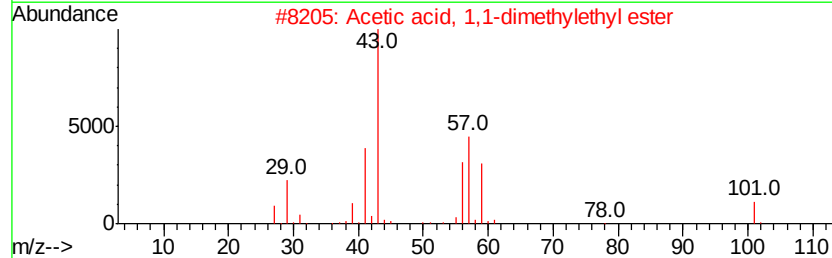
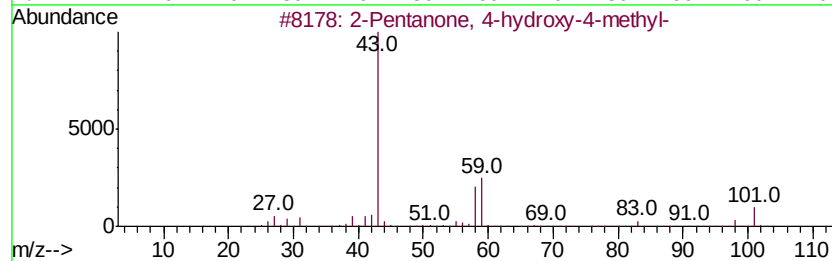
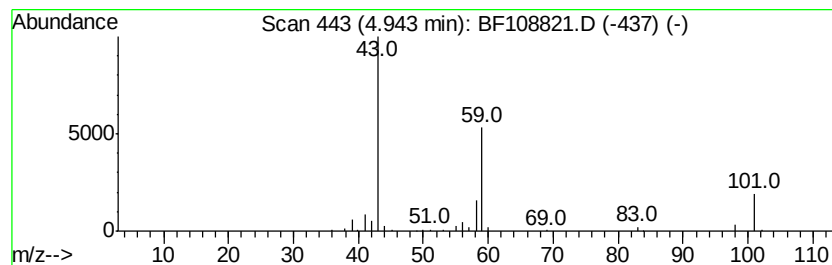
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.94	2.49 ng	213002	1,4-Dichlorobenzene-d4	6.74

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
3		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	10
4		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5		(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9



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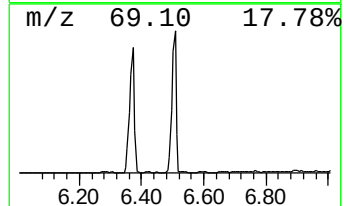
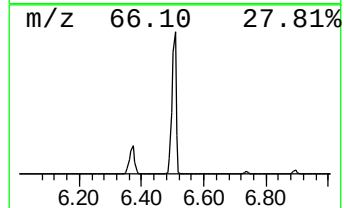
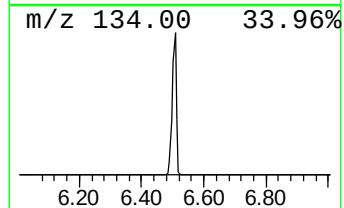
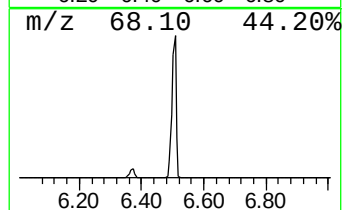
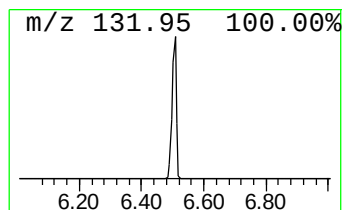
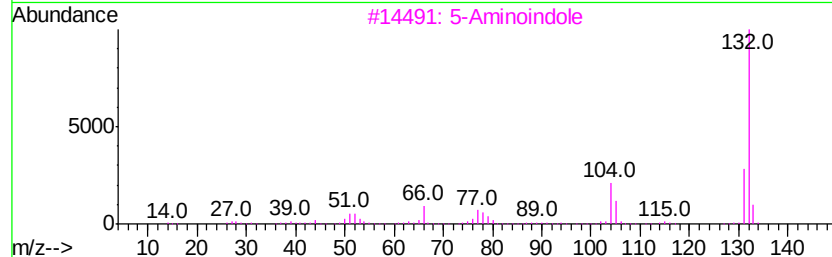
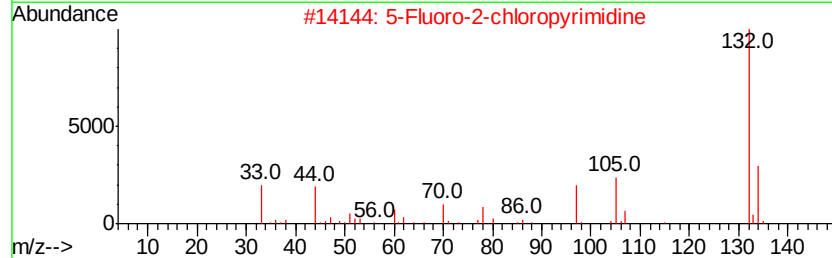
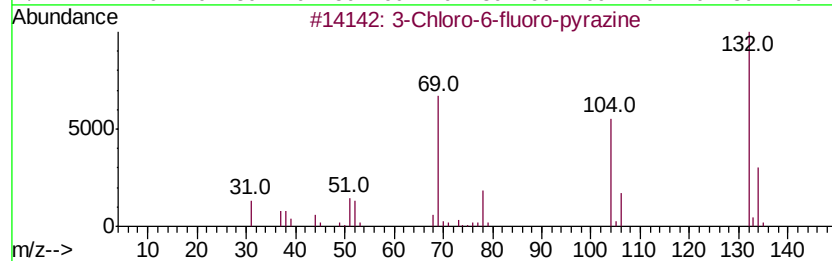
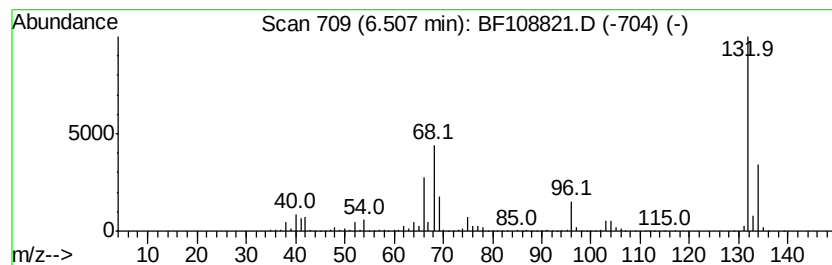
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 2 unknown6.51 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.51	59.74 ng	5103020	1,4-Dichlorobenzene-d4	6.74

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
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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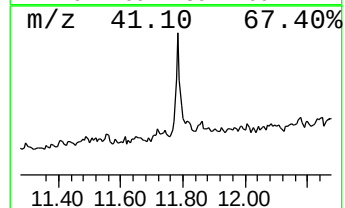
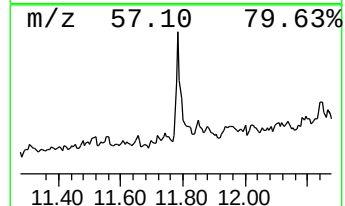
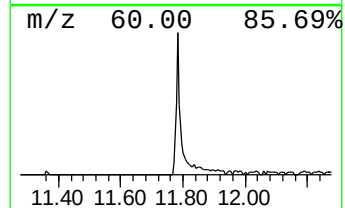
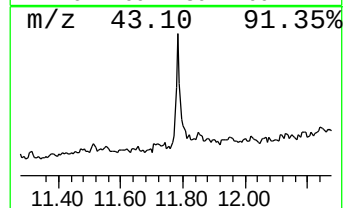
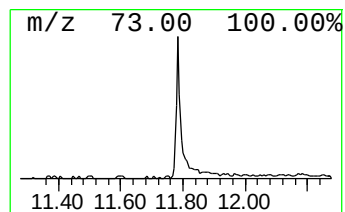
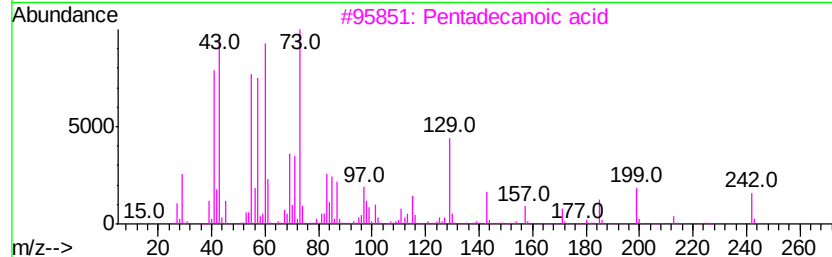
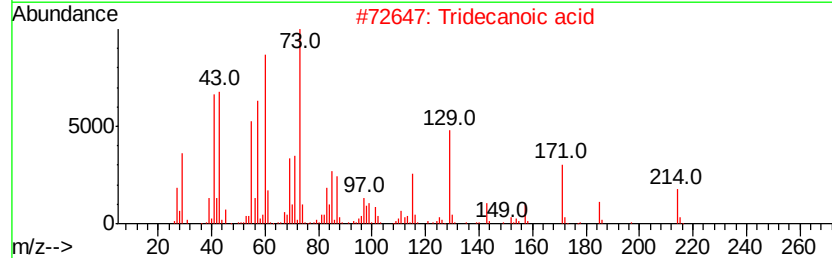
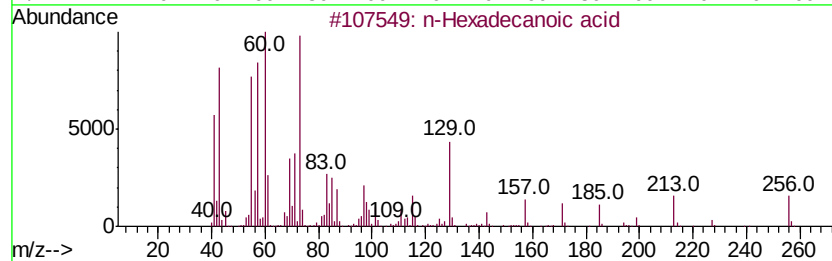
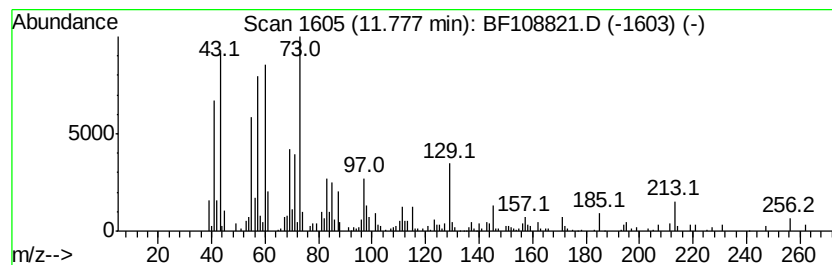
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.78	3.59 ng	303622	Phenanthrene-d10	11.24

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	91
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	83
5		n-Decanoic acid	172	C10H20O2	000334-48-5	76



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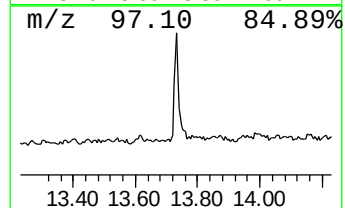
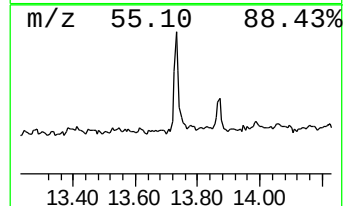
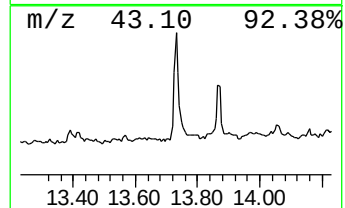
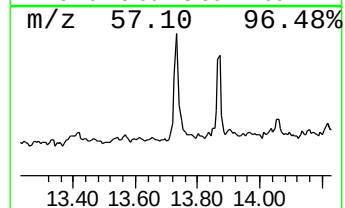
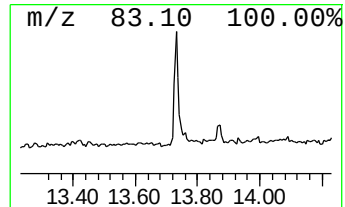
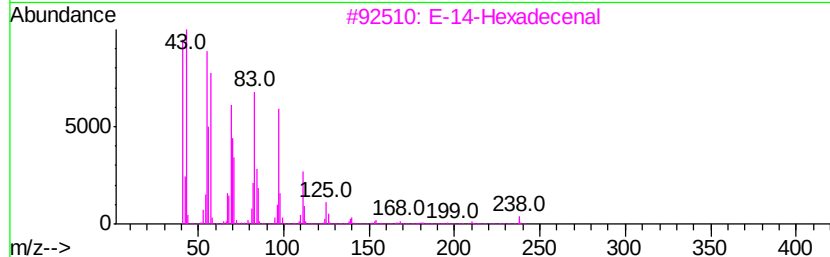
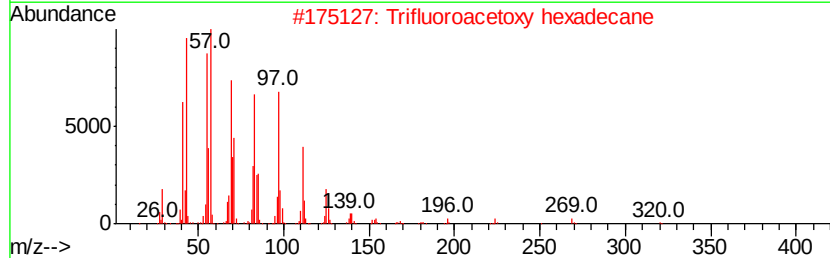
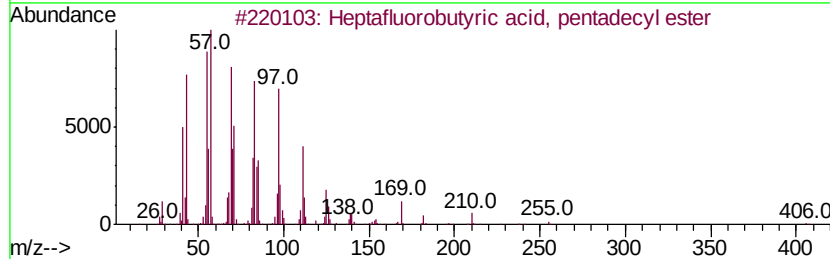
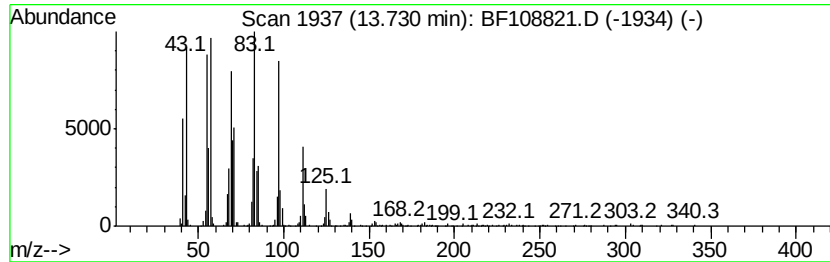
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TIC Integration Parameters: LSCINT.P

Peak Number 5 Heptafluorobutyric acid, pe... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.73	6.08 ng	593221	Chrysene-d12	13.87

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94
2		Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	93
3		E-14-Hexadecenal	238	C16H30O	330207-53-9	92
4		9-Eicosene, (E)-	280	C20H40	074685-29-3	91
5		Behenic alcohol	326	C22H46O	000661-19-8	91



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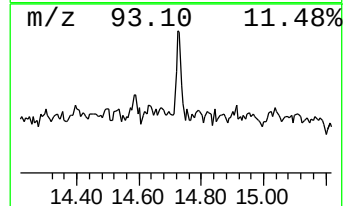
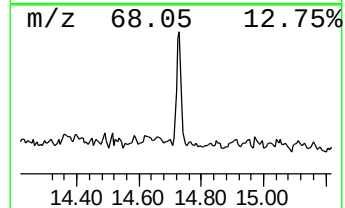
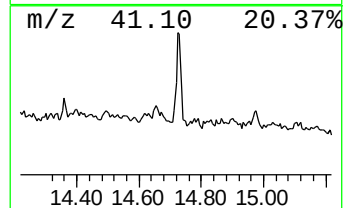
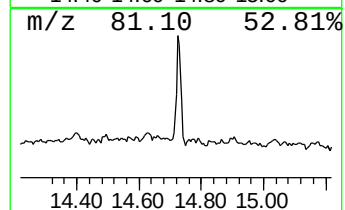
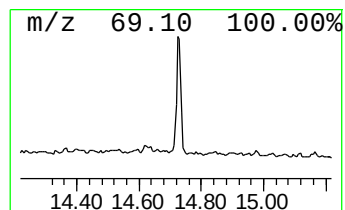
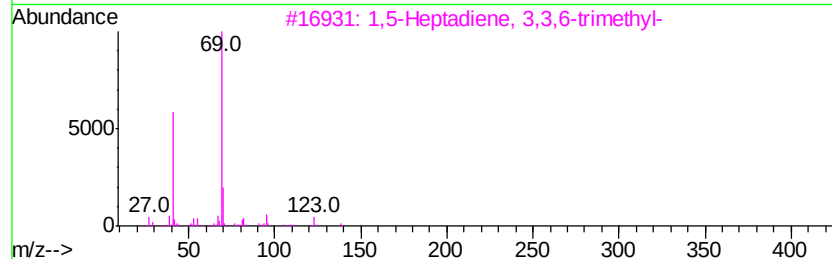
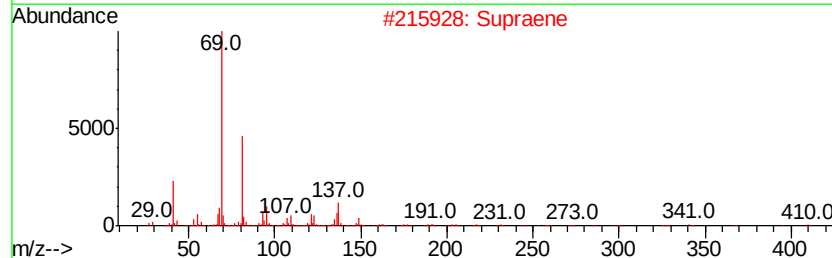
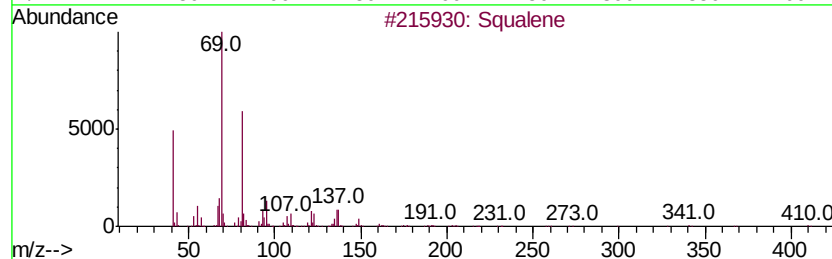
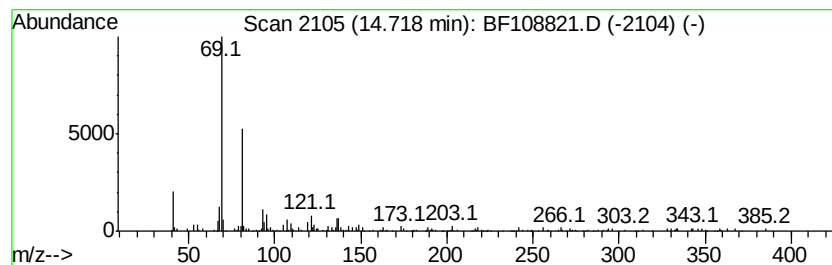
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Peak Number 6 Squalene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.72	4.64 ng	303136	Perylene-d12	15.27

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		1,5-Heptadiene, 3,3,6-trimethyl-	138	C10H18	035387-63-4	64
4		2,6,10-Dodecatrien-1-ol, 3,7,11-...	264	C17H28O2	004128-17-0	64
5		Trideca-1,3,7,11-tetraene-1,1-di...	268	C18H24N2	1000159-88-9	53



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF090518\
Data File : BF108821.D
Acq On : 6 Sep 2018 12:58
Operator : JU/SJ
Sample : J4724-14
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
EP1-SUT-8USTS-W

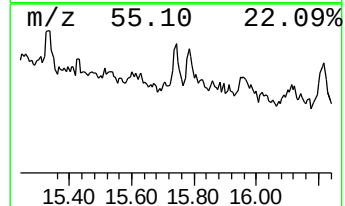
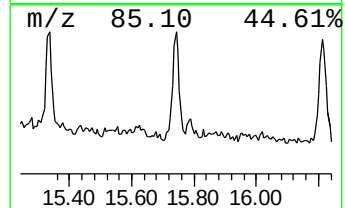
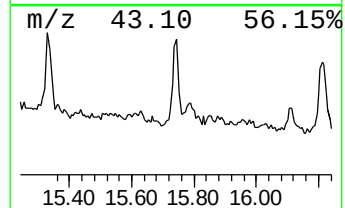
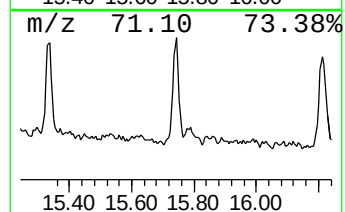
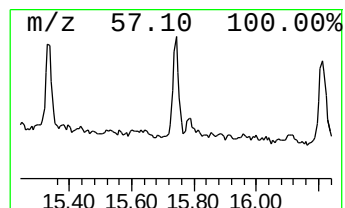
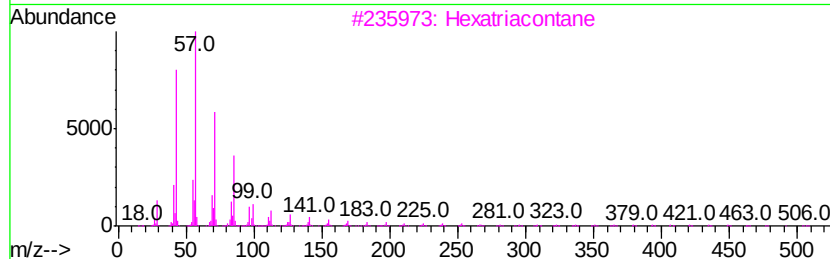
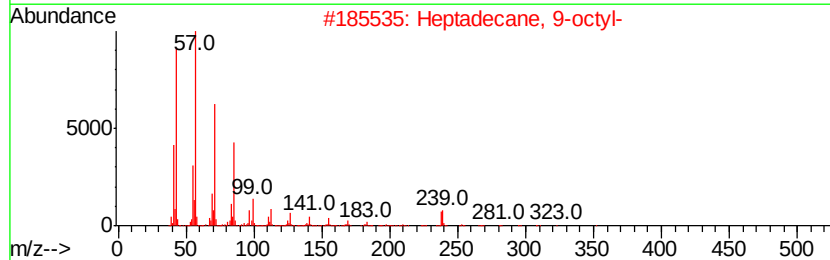
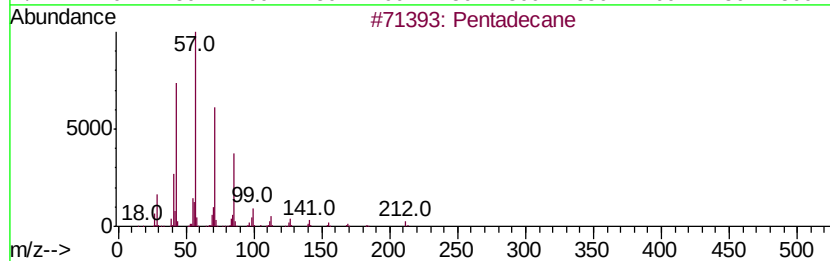
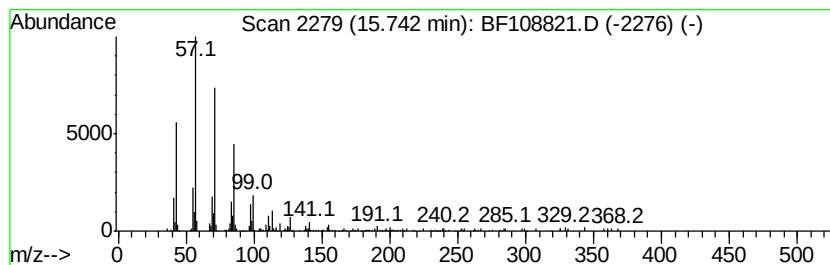
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Pentadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.74	2.36 ng	154598	Perylene-d12	15.27

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentadecane	212	C15H32	000629-62-9	93
2		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
3		Hexatriacontane	507	C36H74	000630-06-8	91
4		Heptadecane	240	C17H36	000629-78-7	90
5		Tetratetracontane	619	C44H90	007098-22-8	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF090518\
Data File : BF108821.D
Acq On : 6 Sep 2018 12:58
Operator : JU/SJ
Sample : J4724-14
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
EP1-SUT-8USTS-W

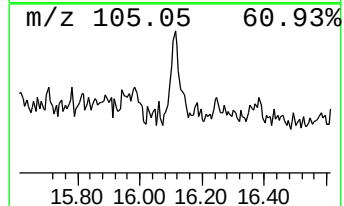
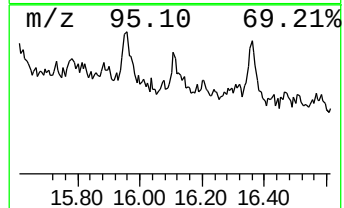
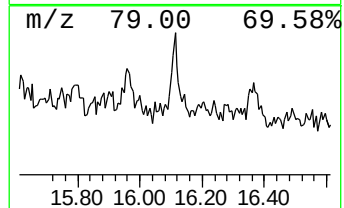
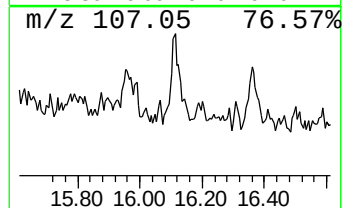
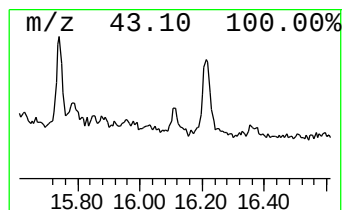
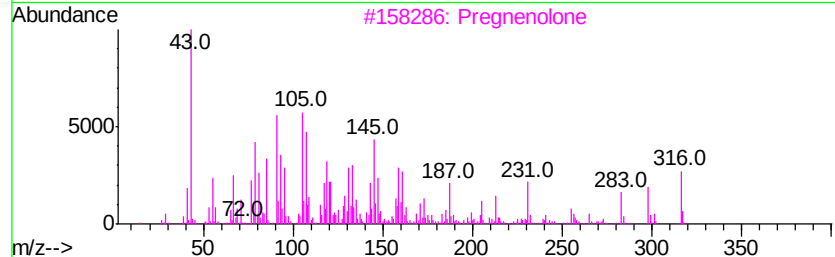
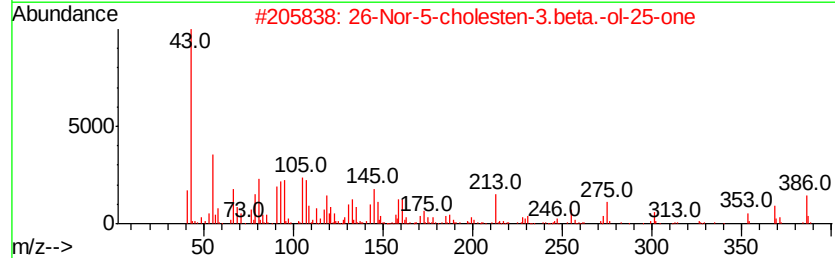
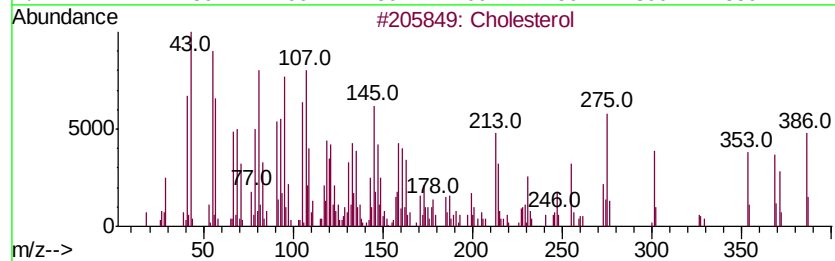
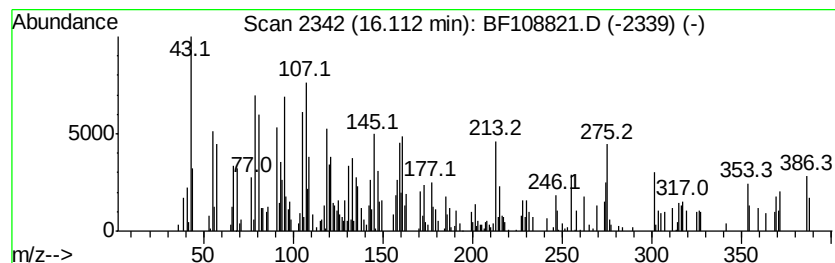
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Cholesterol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.11	2.82 ng	184187	Perylene-d12	15.27

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cholesterol	386	C27H46O	000057-88-5	95
2		26-Nor-5-cholesten-3.beta.-ol-25...	386	C26H42O2	007494-34-0	94
3		Pregnenolone	316	C21H32O2	000145-13-1	42
4		(3E,5E,7E)-6-Methyl-8-(2,6,6-tri...	258	C18H26O	017974-57-1	30
5		Cholest-4-en-3-ol	386	C27H46O	014597-42-3	15



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF090518\
Data File : BF108821.D
Acq On : 6 Sep 2018 12:58
Operator : JU/SJ
Sample : J4724-14
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
EP1-SUT-8USTS-W

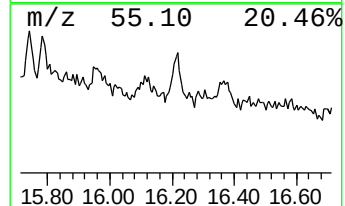
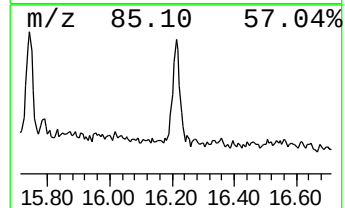
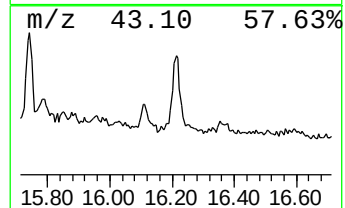
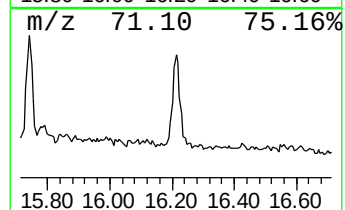
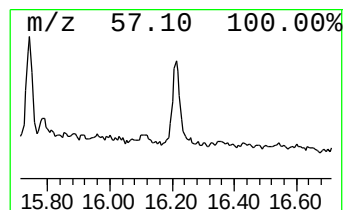
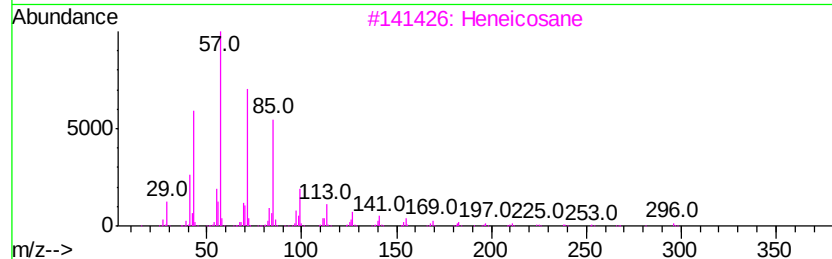
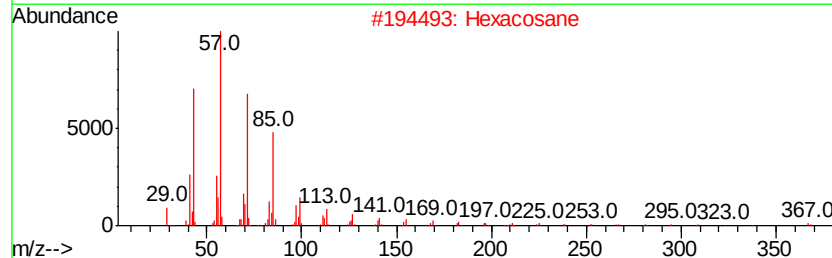
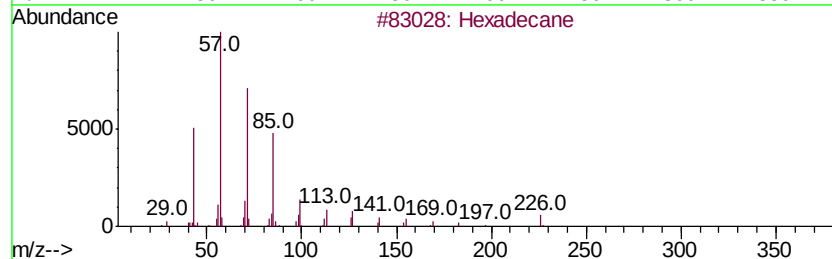
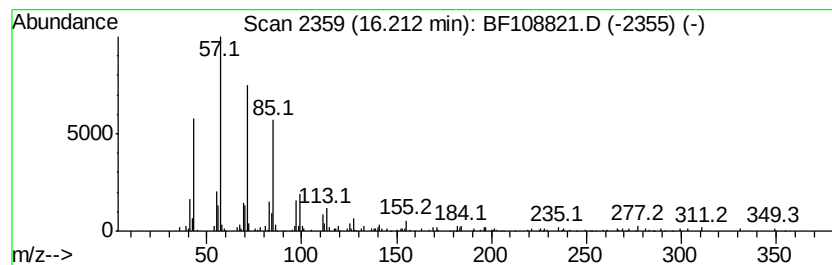
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF090518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Hexadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.21	2.78 ng	182031	Perylene-d12	15.27

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecane	226	C16H34	000544-76-3	93
2		Hexacosane	366	C26H54	000630-01-3	91
3		Heneicosane	296	C21H44	000629-94-7	91
4		Heptacosane, 1-chloro-	414	C27H55Cl	062016-79-9	90
5		Heptacosane	380	C27H56	000593-49-7	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF090518\
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Sample : J4724-14
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
EP1-SUT-8USTS-W

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF090518.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...	4.94	2.5	ng	213002	1	6.74	1708540	20.0
unknown6.51	6.51	59.7	ng	5103020	1	6.74	1708540	20.0
n-Hexadecanoic acid	11.78	3.6	ng	303622	4	11.24	1693570	20.0
Heptafluorobutyri...	13.73	6.1	ng	593221	5	13.87	1951480	20.0
Squalene	14.72	4.6	ng	303136	6	15.27	1307420	20.0
Pentadecane	15.74	2.4	ng	154598	6	15.27	1307420	20.0
Cholesterol	16.11	2.8	ng	184187	6	15.27	1307420	20.0
Hexadecane	16.21	2.8	ng	182031	6	15.27	1307420	20.0