

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF073018\
 Data File : BF107819.D
 Acq On : 30 Jul 2018 23:53
 Operator : JU/SJ
 Sample : J4164-08
 Misc :
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-4(7-9)

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-BF073018.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	5.201	482	487	498	rBV	529558	776109	16.72%	1.842%
2	5.601	551	555	591	rBV	3059625	4383106	94.43%	10.401%
3	6.601	721	725	744	rBV	2628374	4310463	92.87%	10.228%
4	6.737	744	748	770	rVB	3694749	4530096	97.60%	10.749%
5	6.960	783	786	808	rVB	797933	1127893	24.30%	2.676%
6	7.113	808	812	833	rBV	3047662	3473895	74.84%	8.243%
7	7.525	878	882	906	rBV	1821481	2908684	62.67%	6.902%
8	8.242	1000	1004	1035	rBV	1173327	1526661	32.89%	3.623%
9	9.313	1181	1186	1208	rBV	4120381	4641523	100.00%	11.014%
10	9.707	1249	1253	1264	rBV	224250	232064	5.00%	0.551%
11	10.001	1298	1303	1319	rBV	1449079	1534505	33.06%	3.641%
12	10.795	1434	1438	1451	rBV	2235815	2875641	61.95%	6.824%
13	11.495	1553	1557	1566	rBV	1169967	1426233	30.73%	3.384%
14	12.001	1639	1643	1647	rBV	70954	88492	1.91%	0.210%
15	12.713	1760	1764	1773	rBV	102826	157650	3.40%	0.374%
16	12.925	1797	1800	1801	rBV	54277	47046	1.01%	0.112%
17	12.948	1801	1804	1808	rVB	110345	123055	2.65%	0.292%
18	13.077	1822	1826	1837	rBV	3503788	3765383	81.12%	8.935%
19	13.624	1916	1919	1922	rBV	97879	95694	2.06%	0.227%
20	13.954	1971	1975	1980	rBV	404975	475000	10.23%	1.127%
21	14.148	2003	2008	2021	rBV	1255789	1788402	38.53%	4.244%
22	14.271	2026	2029	2032	rBV	135496	123545	2.66%	0.293%
23	14.577	2078	2081	2090	rVB4	198438	311277	6.71%	0.739%
24	14.895	2132	2135	2139	rBV2	121149	124789	2.69%	0.296%
25	14.977	2146	2149	2152	rVB	114655	125220	2.70%	0.297%
26	15.248	2193	2195	2200	rVB	133808	147672	3.18%	0.350%
27	15.683	2264	2269	2276	rBV	692743	1022361	22.03%	2.426%

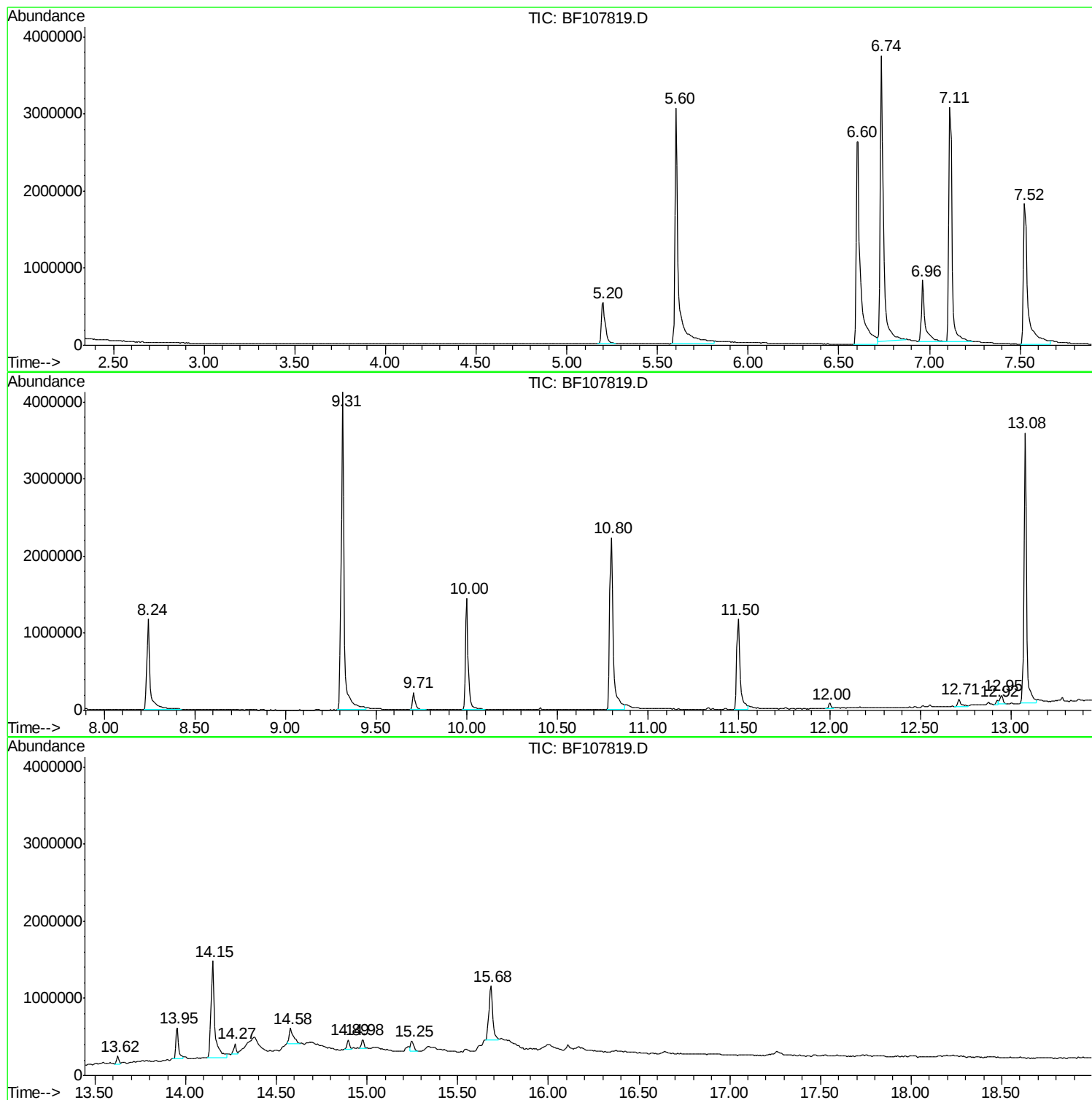
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF073018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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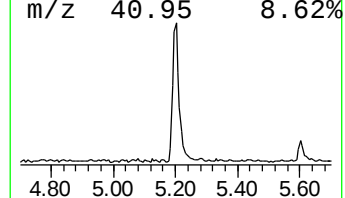
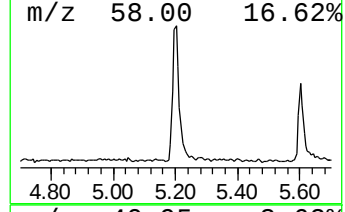
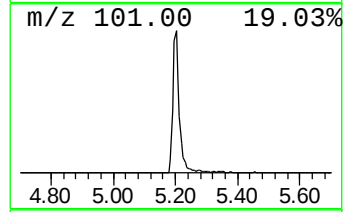
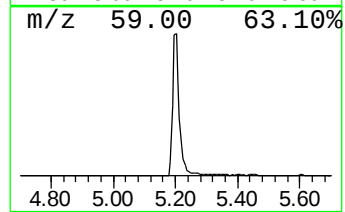
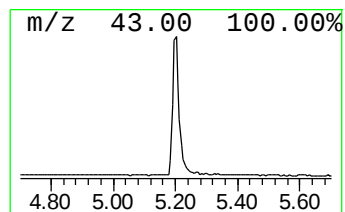
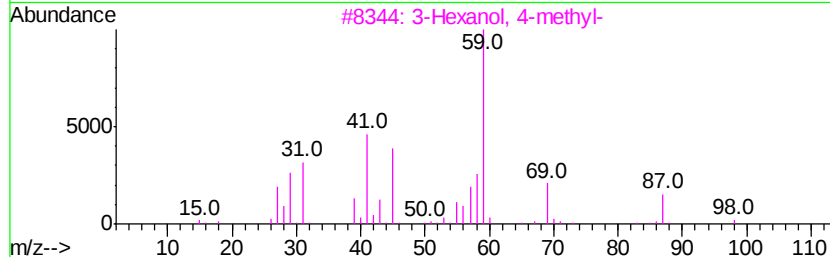
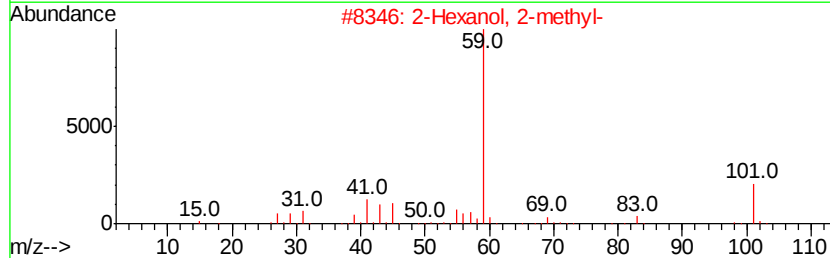
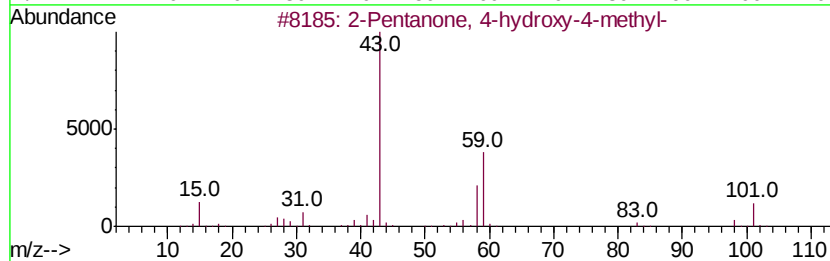
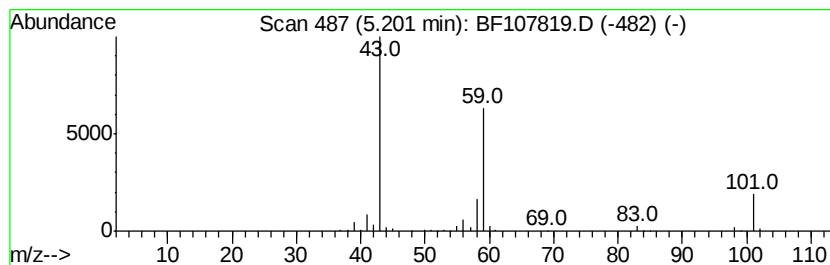
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.20	13.76 ng	776109	1,4-Dichlorobenzene-d4	6.96

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
3			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
4			Propane, 2-methyl-2-(1-methylethyl)-	116	C7H16O	017348-59-3	28
5			Acetic acid, cyano-, 1,1-dimethyl-	141	C7H11NO2	001116-98-9	23



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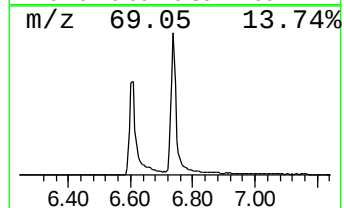
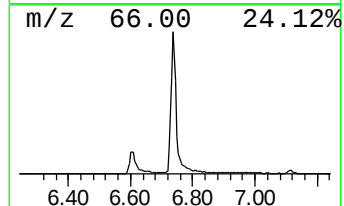
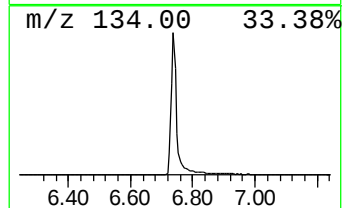
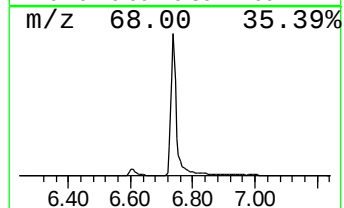
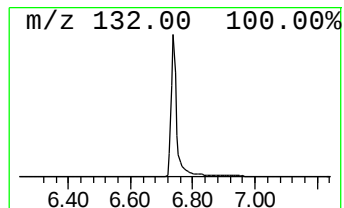
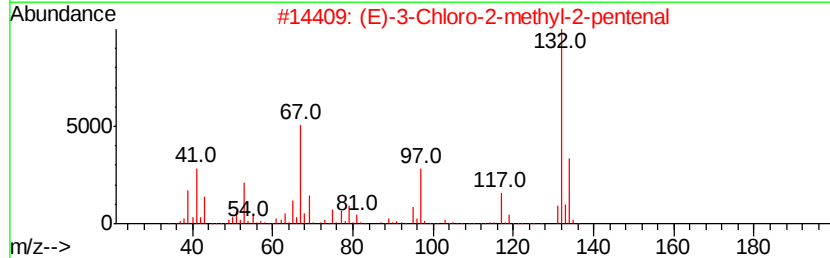
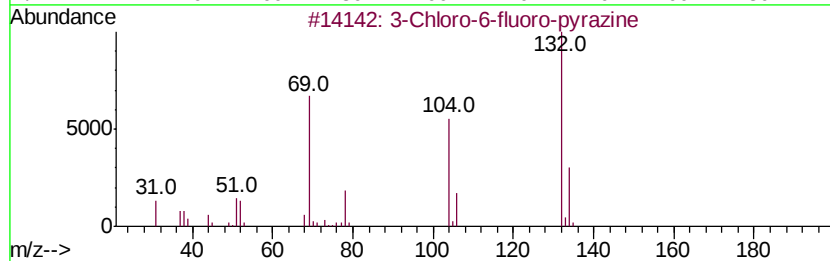
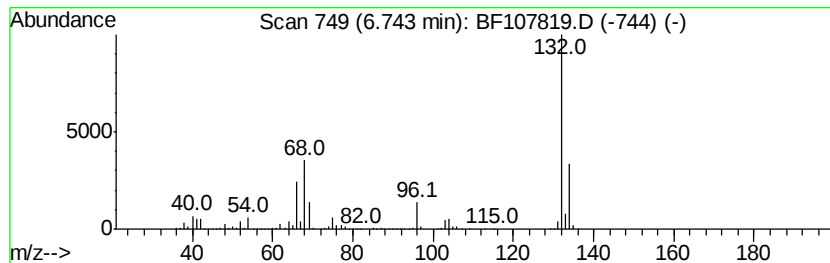
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Peak Number 2 unknown6.74 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.74	80.33 ng	4530100	1,4-Dichlorobenzene-d4	6.96

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	16
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	10
4		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5		(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	9



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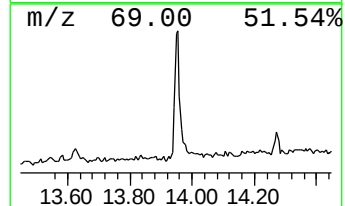
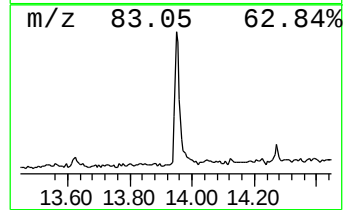
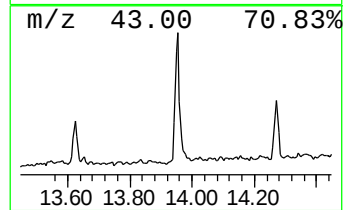
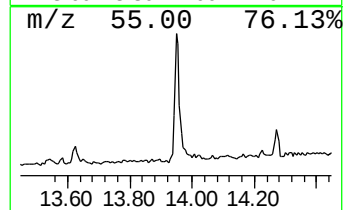
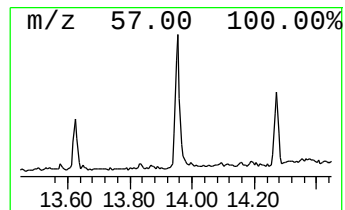
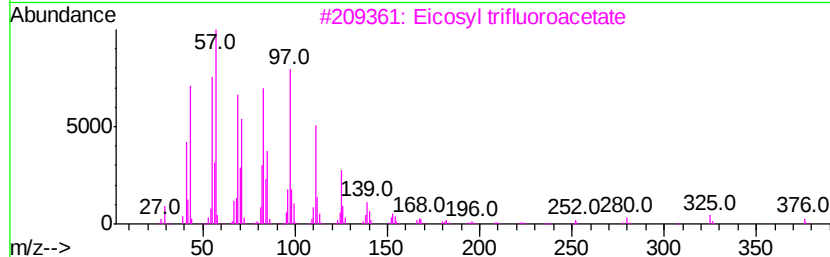
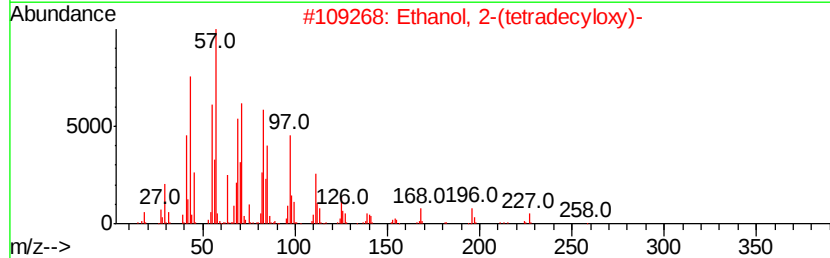
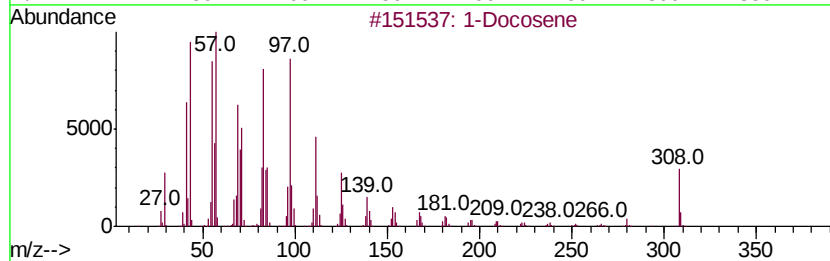
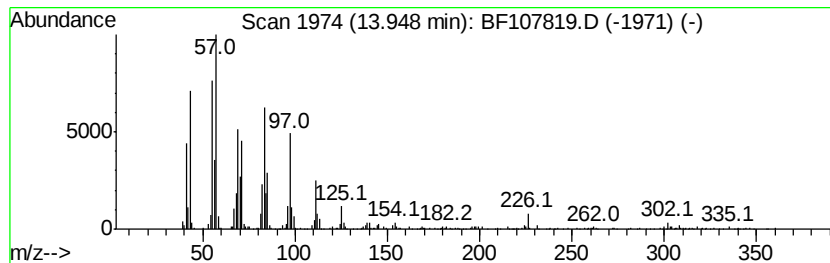
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Peak Number 5 1-Docosene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.95	5.31 ng	475000	Chrysene-d12	14.15

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene		308	C22H44	001599-67-3	94
2	Ethanol, 2-(tetradecyloxy)-		258	C16H34O2	002136-70-1	91
3	Eicosyl trifluoroacetate		394	C22H41F3O2	1000351-75-2	91
4	Oxalic acid, isobutyl hexadecyl ...		370	C22H42O4	1000309-38-1	91
5	1-Hexadecanesulfonyl chloride		324	C16H33ClO2S	038775-38-1	91



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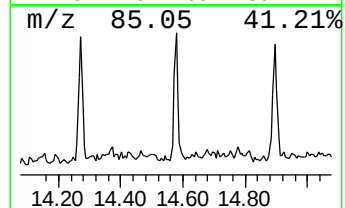
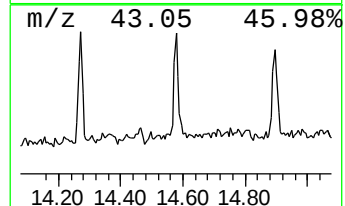
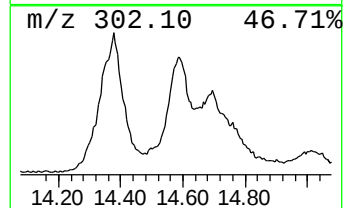
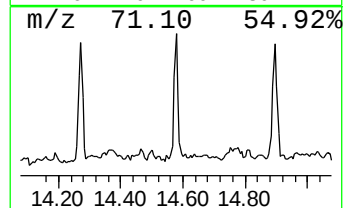
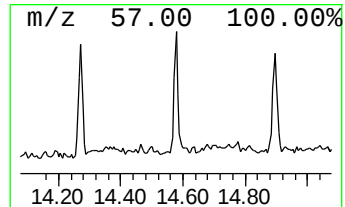
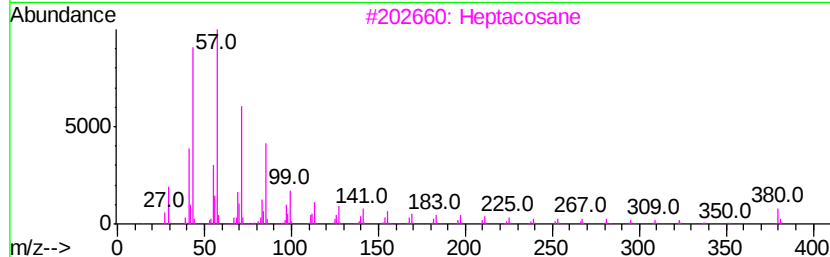
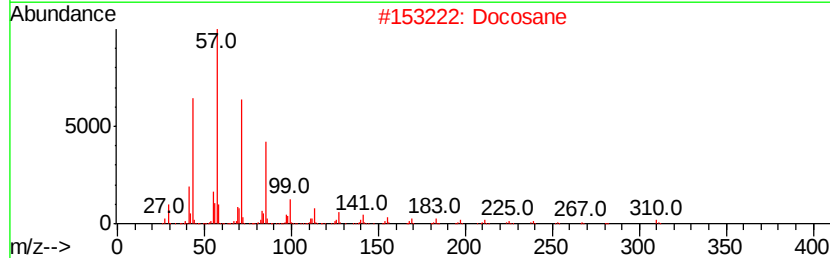
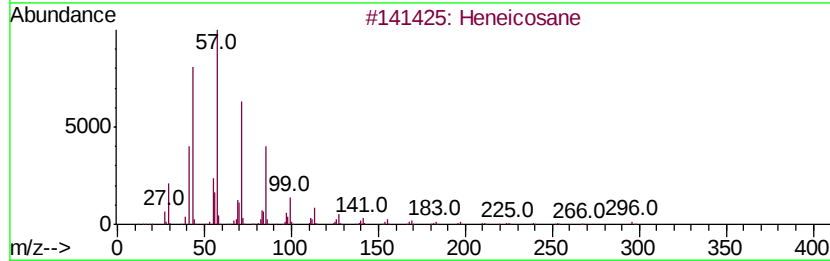
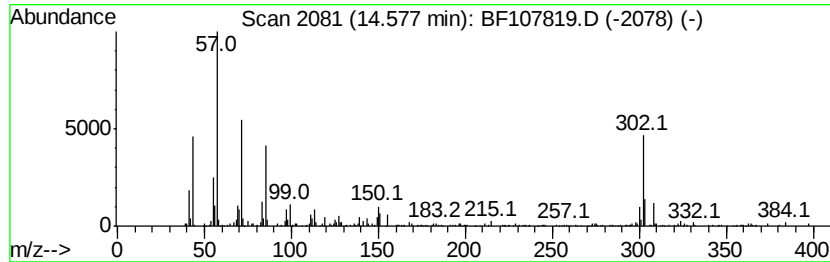
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 6 Heneicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.58	3.48 ng	311277	Chrysene-d12	14.15

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane		296	C21H44	000629-94-7	64
2	Docosane		310	C22H46	000629-97-0	55
3	Heptacosane		380	C27H56	000593-49-7	55
4	Tricosane		324	C23H48	000638-67-5	55
5	Hexacosane		366	C26H54	000630-01-3	50



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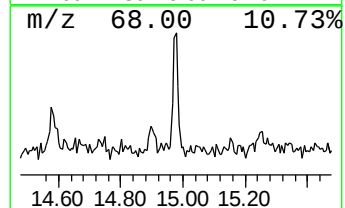
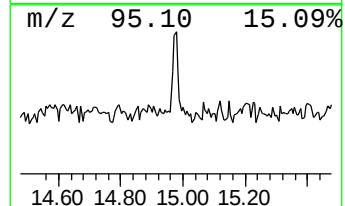
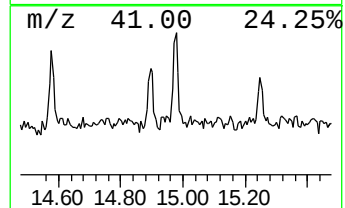
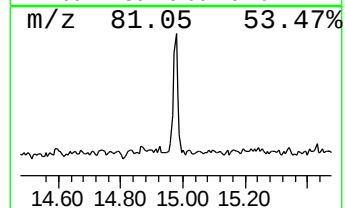
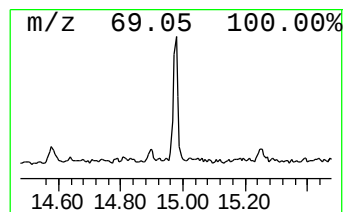
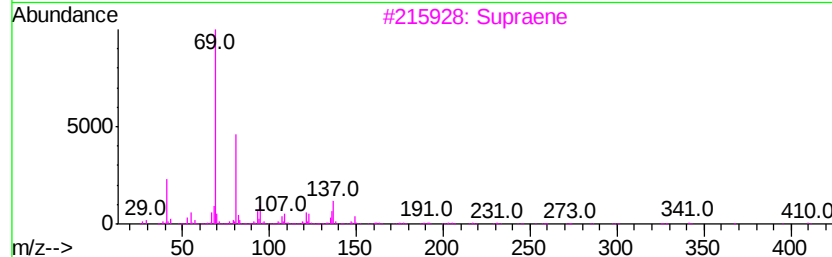
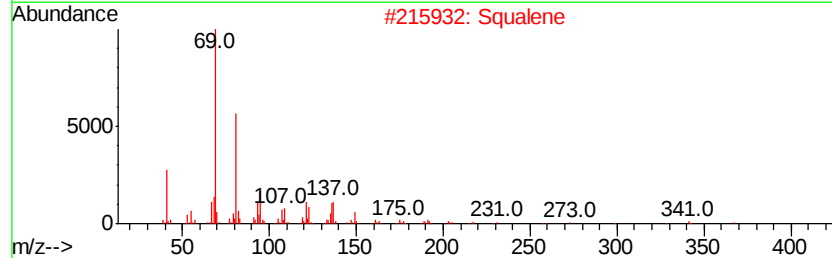
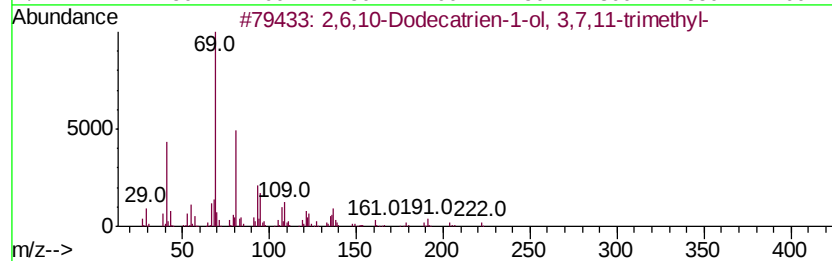
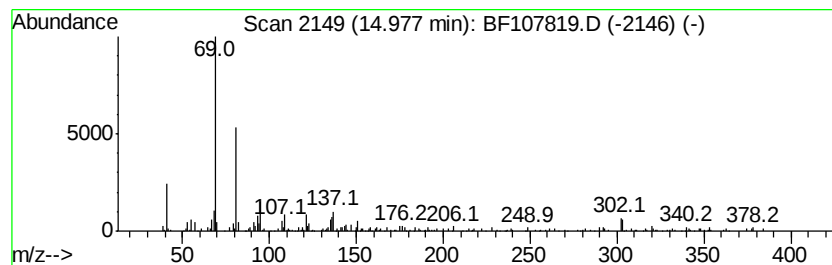
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Peak Number 7 2,6,10-Dodecatrien-1-ol, 3,... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.98	2.45 ng	125220	Perylene-d12	15.68

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	004602-84-0	74
2		Squalene	410	C30H50	000111-02-4	74
3		Supraene	410	C30H50	007683-64-9	72
4		Hexadeca-2,6,10,14-tetraen-1-ol,...	290	C20H34O	007614-21-3	64
5		1-(Phenylthio)-3,7,11-trimethyl-...	314	C21H30S	028413-57-2	64



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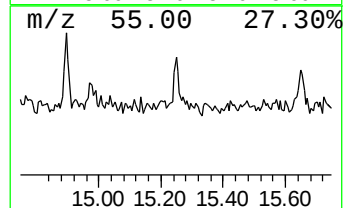
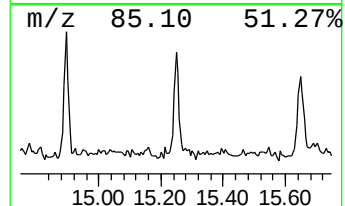
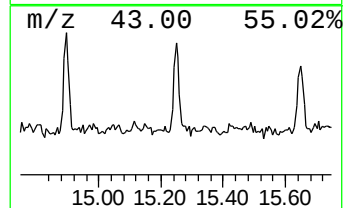
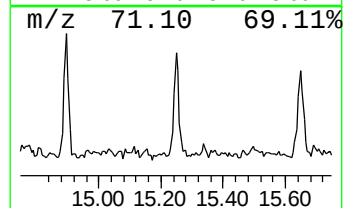
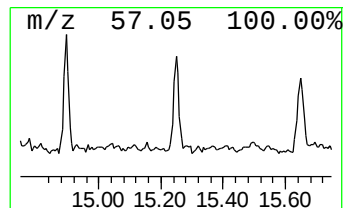
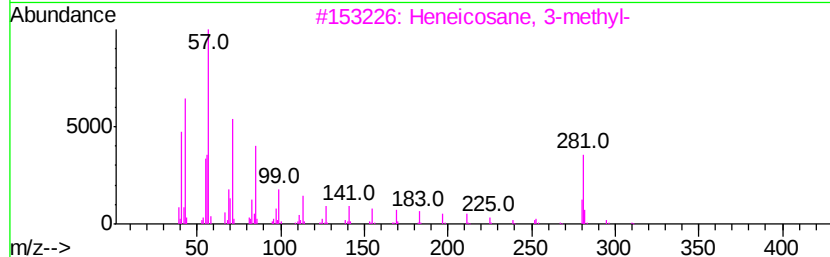
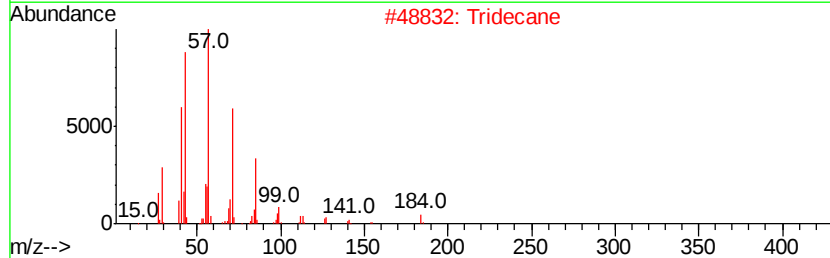
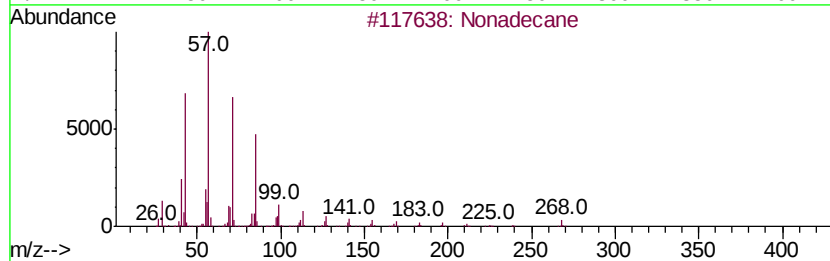
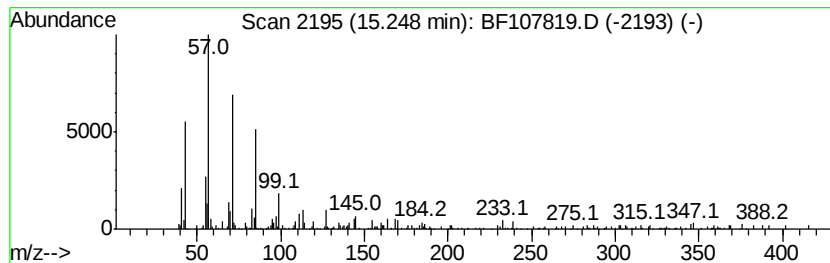
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF073018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Nonadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.25	2.89 ng	147672	Perylene-d12	15.68

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane		268	C19H40	000629-92-5	76
2	Tridecane		184	C13H28	000629-50-5	74
3	Heneicosane, 3-methyl-		310	C22H46	006418-47-9	72
4	Tridecane, 7-propyl-		226	C16H34	055045-09-5	70
5	Heneicosane		296	C21H44	000629-94-7	68



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF073018\
Data File : BF107819.D
Acq On : 30 Jul 2018 23:53
Operator : JU/SJ
Sample : J4164-08
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-4(7-9)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF073018.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...	5.20	13.8	ng	776109	1	6.96	1127890	20.0
unknown6.74	6.74	80.3	ng	4530100	1	6.96	1127890	20.0
1-Docosene	13.95	5.3	ng	475000	5	14.15	1788400	20.0
Heneicosane	14.58	3.5	ng	311277	5	14.15	1788400	20.0
2,6,10-Dodecatric...	14.98	2.5	ng	125220	6	15.68	1022360	20.0
Nonadecane	15.25	2.9	ng	147672	6	15.68	1022360	20.0