

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF082118\
 Data File : BF108366.D
 Acq On : 22 Aug 2018 4:26
 Operator : JU/SJ
 Sample : J4539-06
 Misc :
 ALS Vial : 25 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MS-BASELINE-WATER

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-BF080818.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	2.372	3	6	13	rVB	2730052	3420124	64.97%	9.048%
2	5.242	491	494	505	rVB	110629	132861	2.52%	0.351%
3	5.631	556	560	563	rBV	2361118	2105035	39.99%	5.569%
4	6.619	724	728	732	rBV	1543047	1365156	25.93%	3.612%
5	6.778	750	755	758	rBV	4110807	3849744	73.13%	10.184%
6	7.007	790	794	797	rBV	1216816	1078927	20.49%	2.854%
7	7.060	800	803	807	rVB	96130	73094	1.39%	0.193%
8	7.166	816	821	824	rBV	3816463	3627754	68.91%	9.597%
9	7.572	884	890	893	rBV	3187004	3231801	61.39%	8.550%
10	8.289	1007	1012	1015	rBV	1488354	1273953	24.20%	3.370%
11	8.566	1056	1059	1062	rBV	107837	100234	1.90%	0.265%
12	9.366	1189	1195	1198	rBV	5697346	5264444	100.00%	13.927%
13	9.748	1257	1260	1264	rBV	333508	286231	5.44%	0.757%
14	10.048	1305	1311	1315	rBV2	1455684	1311564	24.91%	3.470%
15	10.454	1377	1380	1385	rVB	68578	66634	1.27%	0.176%
16	10.842	1442	1446	1455	rBV	2726690	2701165	51.31%	7.146%
17	11.548	1559	1566	1573	rVB	1151315	1148727	21.82%	3.039%
18	12.030	1645	1648	1650	rBV2	64156	77976	1.48%	0.206%
19	12.795	1775	1778	1782	rVB	141115	119498	2.27%	0.316%
20	13.130	1831	1835	1839	rBV	3778217	3802432	72.23%	10.059%
21	13.671	1924	1927	1932	rBV2	83006	80514	1.53%	0.213%
22	14.036	1986	1989	1994	rVB4	64682	88008	1.67%	0.233%
23	14.201	2013	2017	2025	rVB	1079952	1013300	19.25%	2.681%
24	14.330	2036	2039	2045	rVB	54990	62159	1.18%	0.164%
25	14.636	2088	2091	2095	rVB2	75914	84322	1.60%	0.223%
26	14.960	2143	2146	2150	rVB	70057	79400	1.51%	0.210%
27	15.048	2157	2161	2165	rVB	112044	131718	2.50%	0.348%
28	15.324	2205	2208	2215	rVB	77153	91366	1.74%	0.242%
29	15.754	2274	2281	2290	rVB	594190	917847	17.43%	2.428%
30	16.212	2355	2359	2366	rVB3	70218	145593	2.77%	0.385%
31	16.765	2450	2453	2460	rVB4	41384	68569	1.30%	0.181%

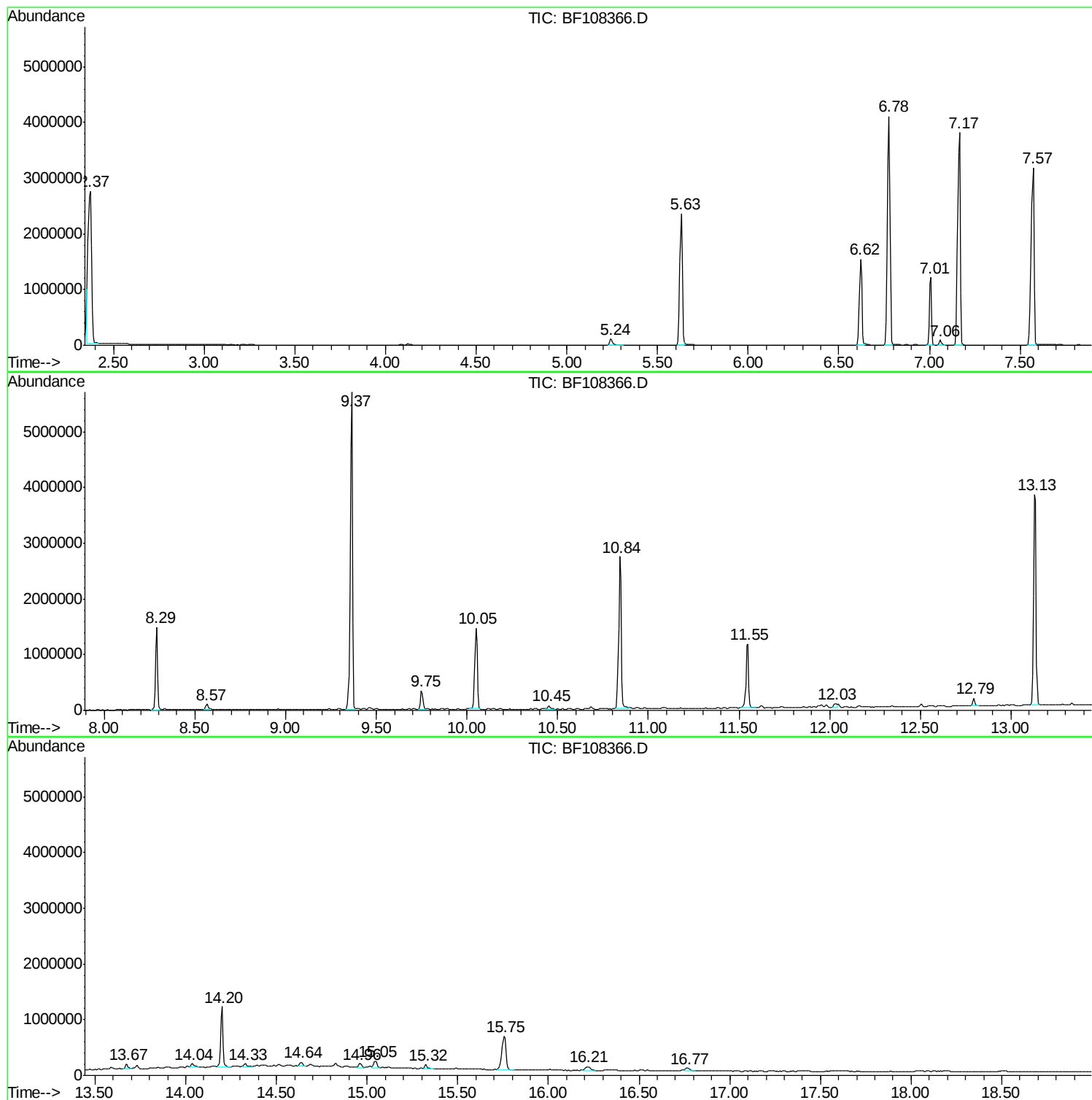
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF080818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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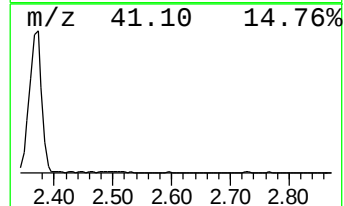
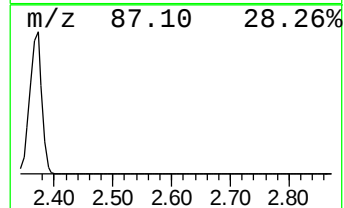
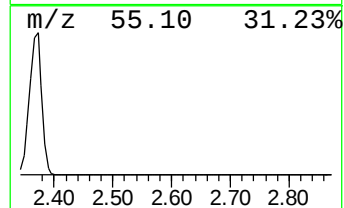
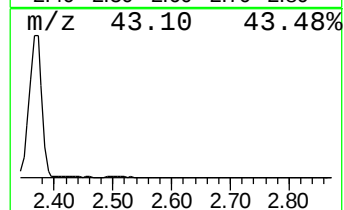
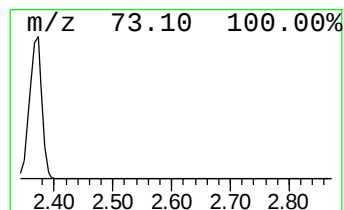
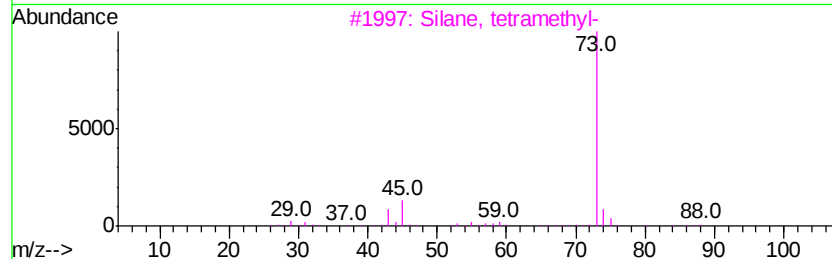
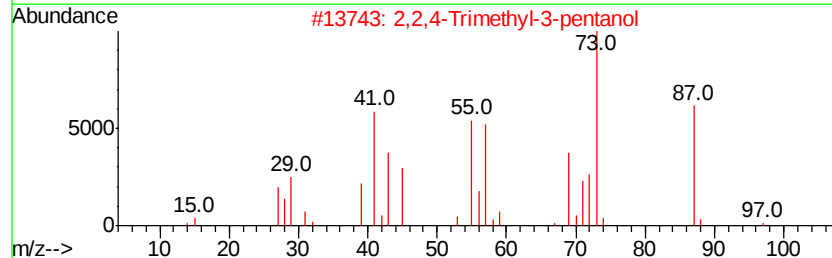
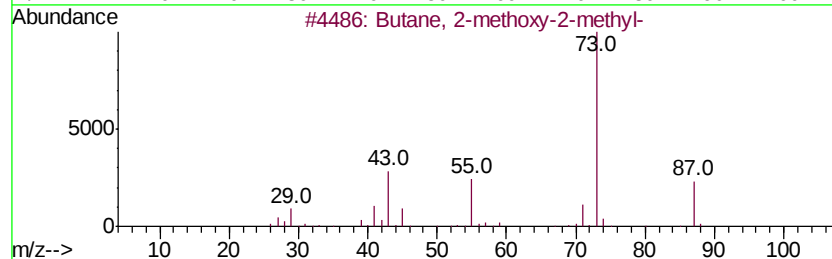
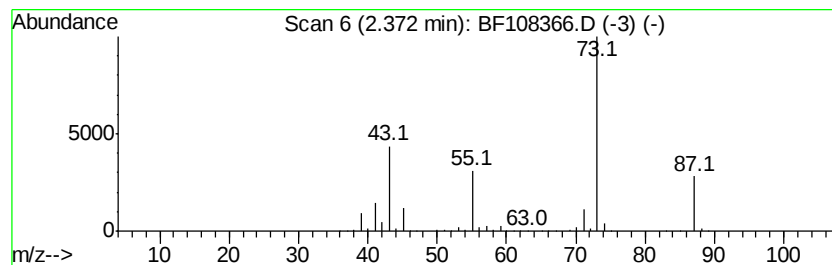
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.37	63.40 ng	3420120	1,4-Dichlorobenzene-d4	7.01

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3		Silane, tetramethyl-	88	C4H12Si	000075-76-3	38
4		3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	37
5		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25



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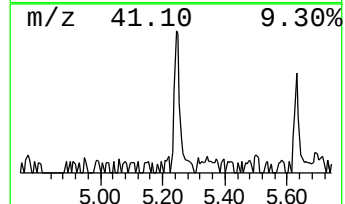
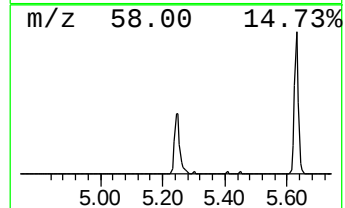
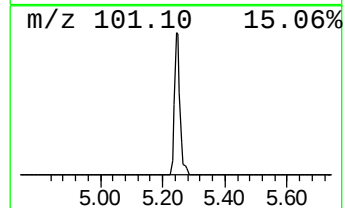
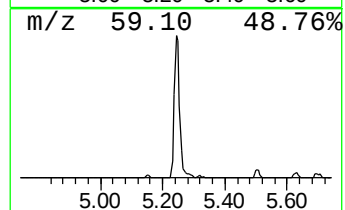
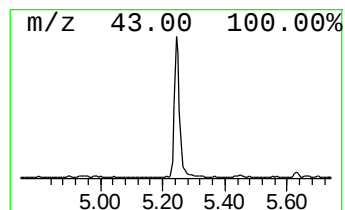
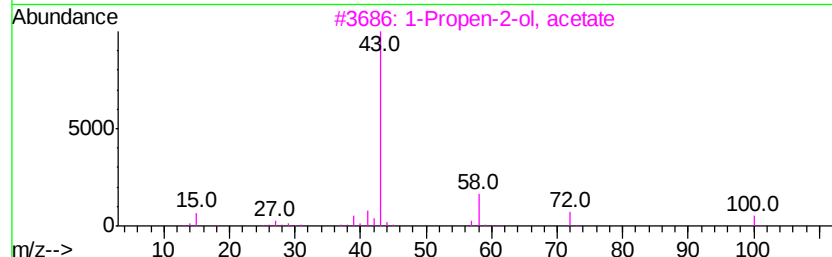
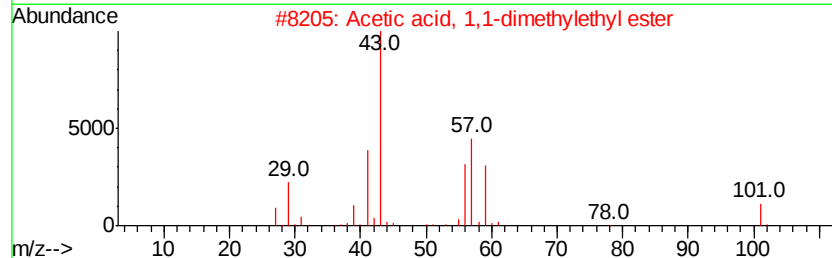
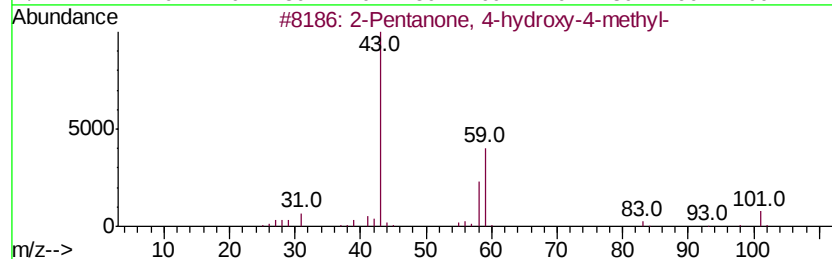
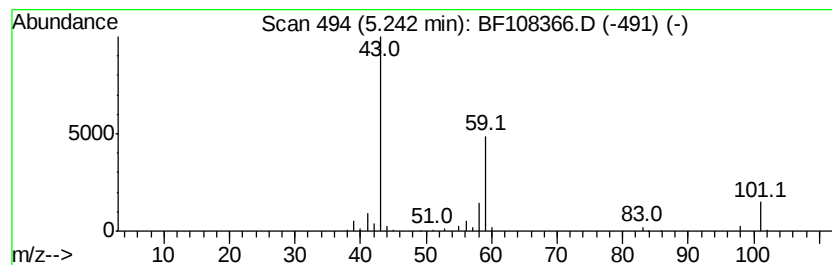
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.24	2.46 ng	132861	1,4-Dichlorobenzene-d4	7.01

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	28
3		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9
4		5-Oxohexanenitrile	111	C6H9NO	010412-98-3	9
5		(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	7



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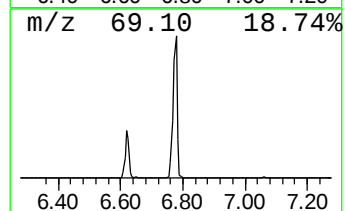
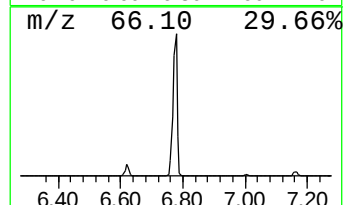
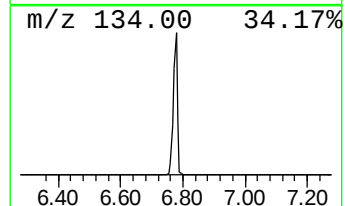
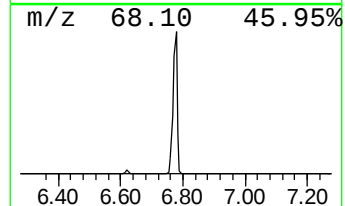
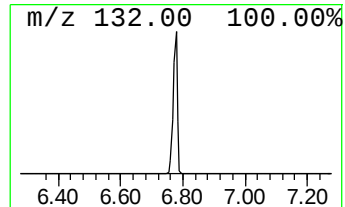
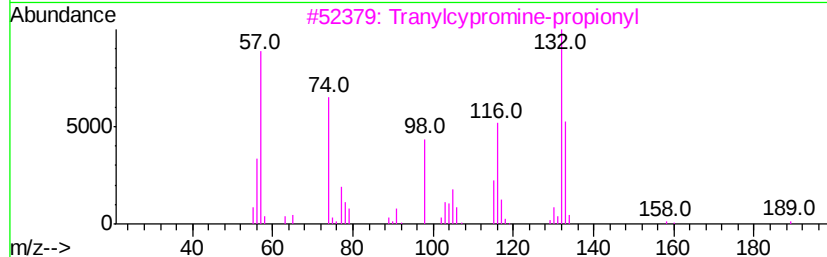
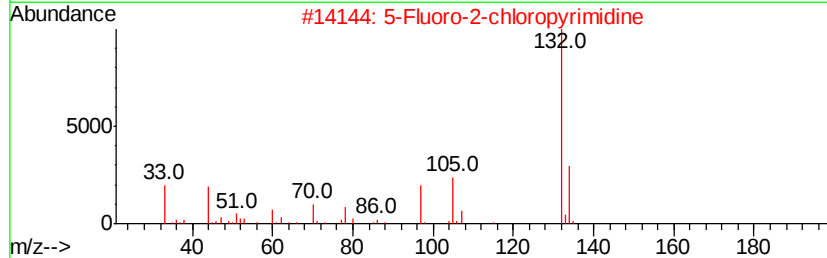
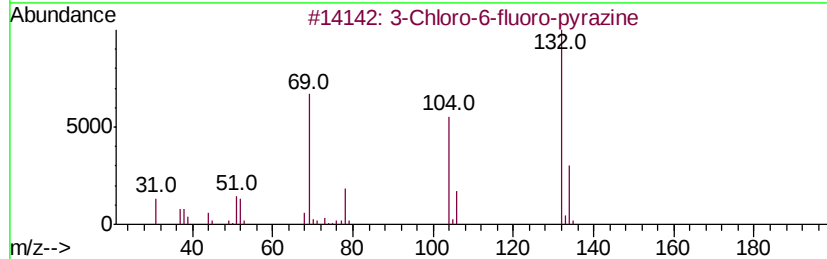
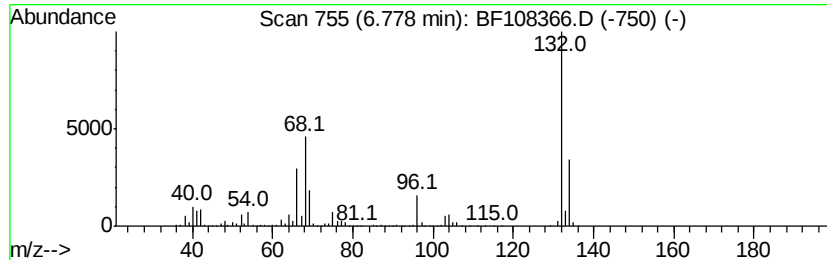
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown6.78 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.78	71.36 ng	3849740	1,4-Dichlorobenzene-d4	7.01

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	10
4		1,2,4-Trifluorobenzene	132	C6H3F3	000367-23-7	9
5		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9



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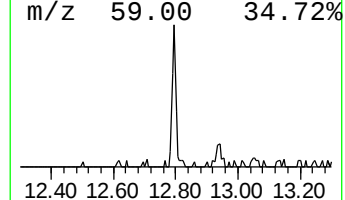
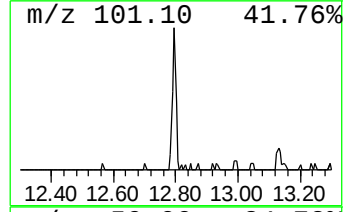
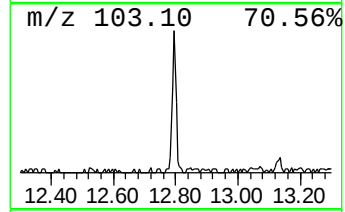
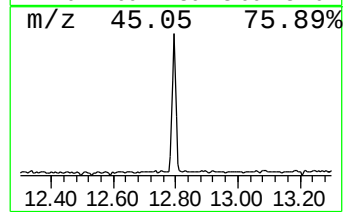
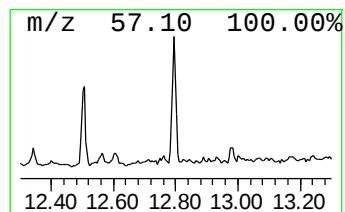
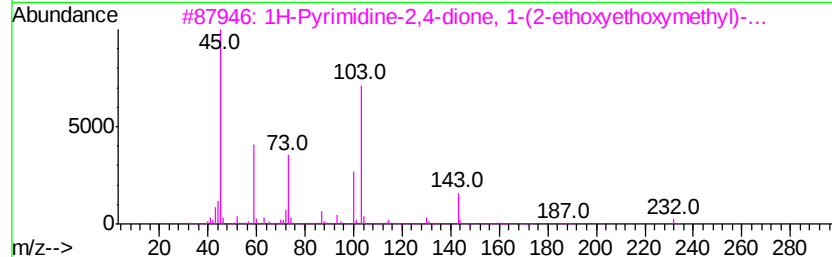
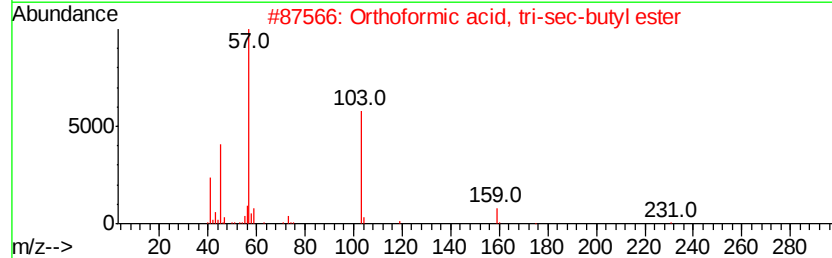
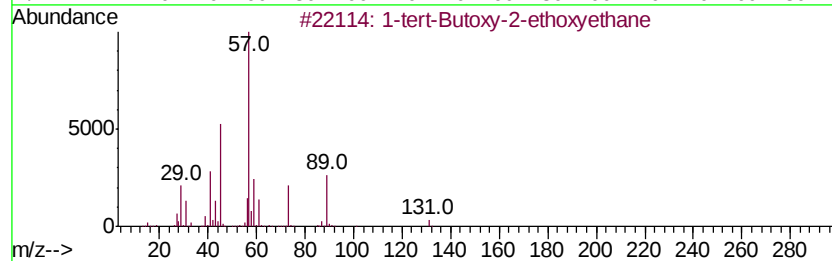
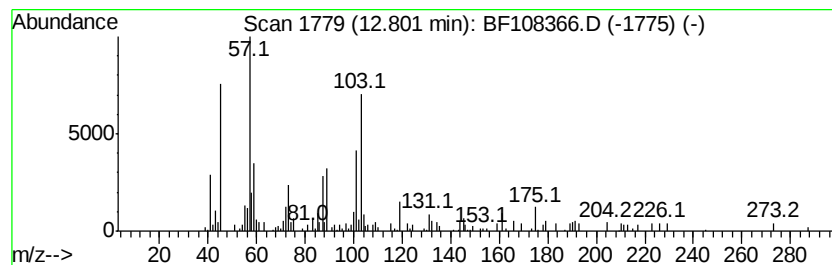
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Peak Number 5 unknown12.80 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.80	2.08 ng	119498	Phenanthrene-d10	11.55

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-tert-Butoxy-2-ethoxyethane	146	C8H18O2	051422-54-9	43
2		Orthoformic acid, tri-sec-butyl ...	232	C13H28O3	016754-48-6	38
3		1H-Pyrimidine-2,4-dione, 1-(2-et...	232	C9H13FN2O4	1000310-13-7	37
4		Di-sec-butyl ether	130	C8H18O	006863-58-7	35
5		Carbonic acid, bis(1-methylpropy...	174	C9H18O3	000623-63-2	27



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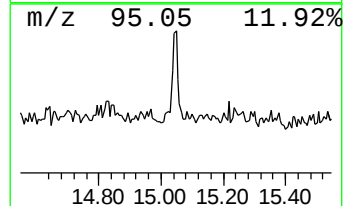
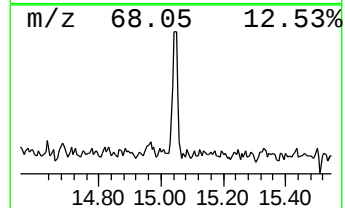
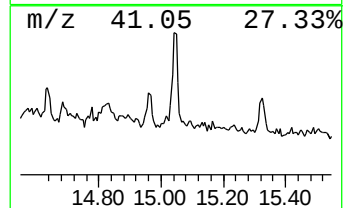
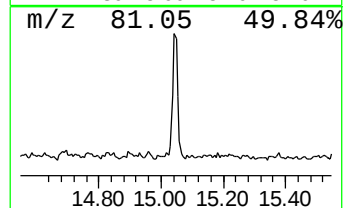
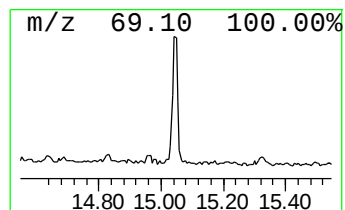
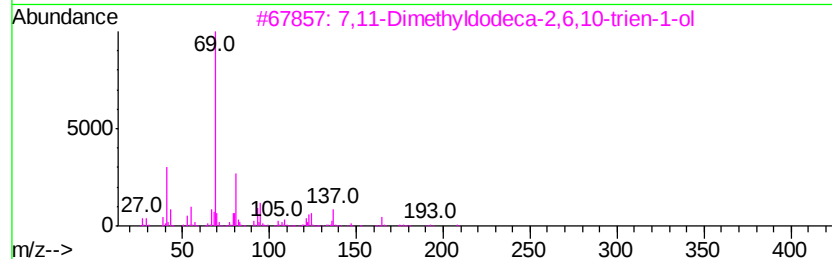
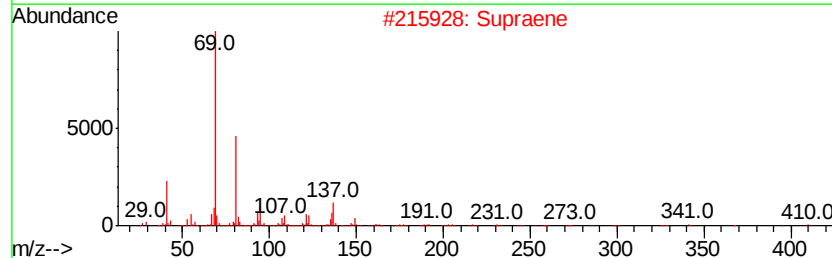
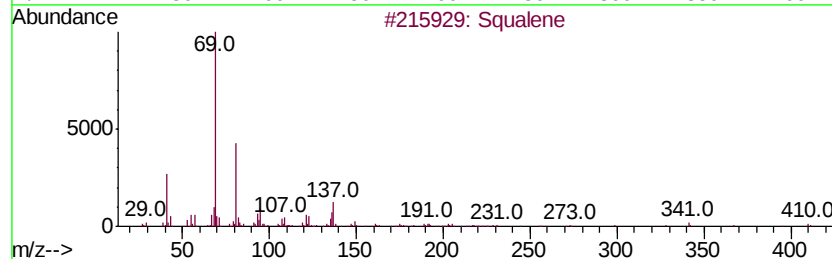
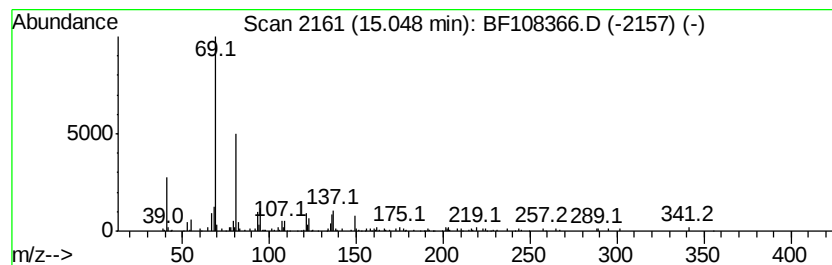
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Peak Number 6 Squalene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.05	2.87 ng	131718	Perylene-d12	15.75	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	87
2	Supraene	410	C30H50	007683-64-9	83
3	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H240	125529-10-4	72
4	(.+/-)-Lavandulol, pentafluorop...	300	C13H17F5O2	1000352-63-1	72
5	1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	72



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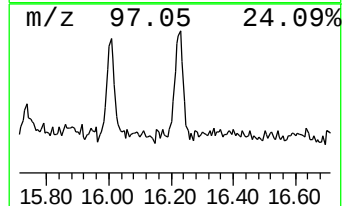
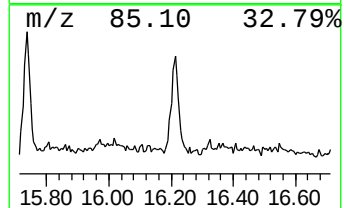
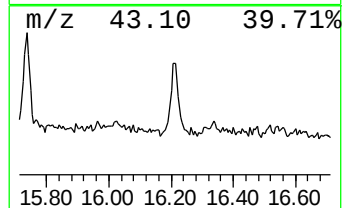
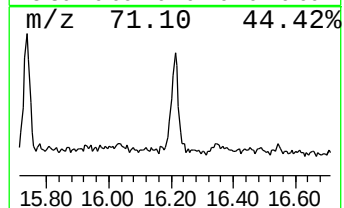
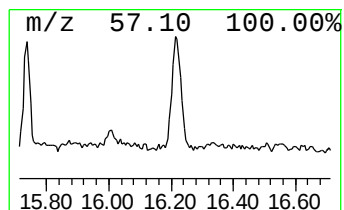
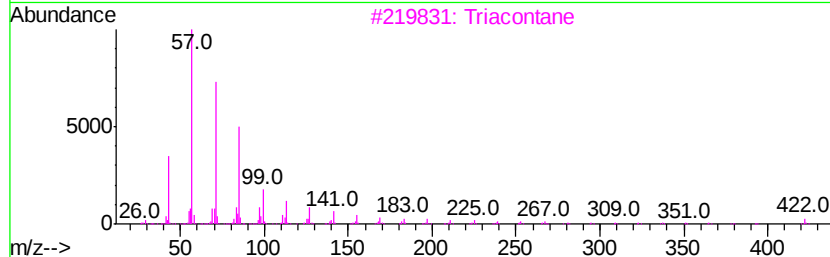
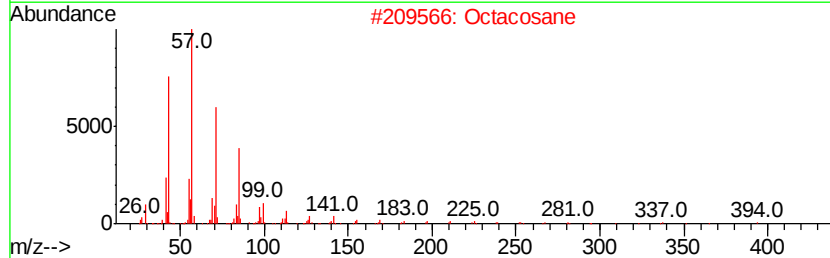
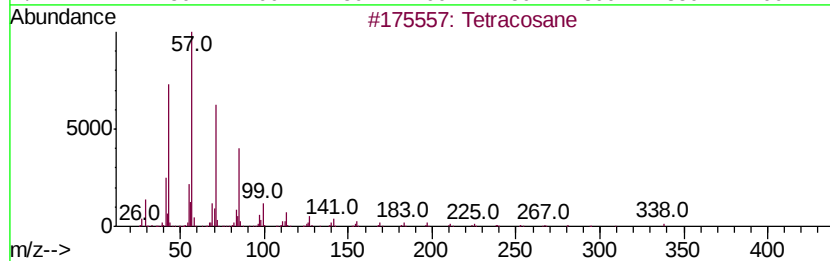
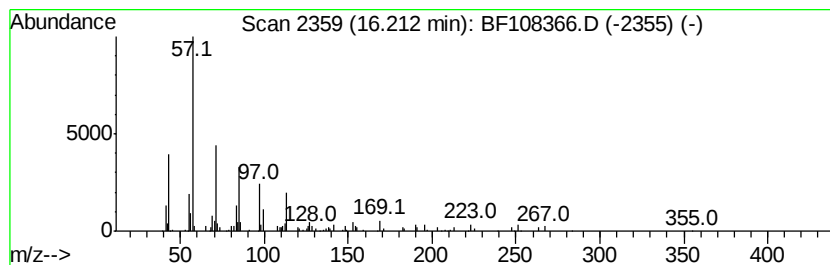
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Tetracosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.21	3.17 ng	145593	Perylene-d12	15.75

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tetracosane	338	C24H50	000646-31-1	53
2		Octacosane	394	C28H58	000630-02-4	53
3		Triacontane	422	C30H62	000638-68-6	53
4		Sulfurous acid, butyl dodecyl ester	306	C16H34O3S	1000309-17-9	53
5		Pentacosane	352	C25H52	000629-99-2	53



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF082118\
Data File : BF108366.D
Acq On : 22 Aug 2018 4:26
Operator : JU/SJ
Sample : J4539-06
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MS-BASELINE-WATER

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.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
Butane, 2-methoxy...	2.37	63.4	ng	3420120	1	7.01	1078930	20.0
2-Pentanone, 4-hy...	5.24	2.5	ng	132861	1	7.01	1078930	20.0
unknown6.78	6.78	71.4	ng	3849740	1	7.01	1078930	20.0
unknown12.80	12.80	2.1	ng	119498	4	11.55	1148730	20.0
Squalene	15.05	2.9	ng	131718	6	15.75	917847	20.0
Tetracosane	16.21	3.2	ng	145593	6	15.75	917847	20.0