

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF082517\
 Data File : BF098036.D
 Acq On : 25 Aug 2017 17:56
 Operator : SJ/JU
 Sample : I4974-01
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 JPS-W1

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:\HPCHEM1\BNA_F\METHODS\8270-BF081517.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	4.934	480	484	492	rVB	651698	686288	19.85%	2.941%
2	5.346	550	554	558	rBV	988875	832001	24.07%	3.566%
3	6.363	723	727	738	rBV	831545	672104	19.44%	2.880%
4	6.504	747	751	754	rBV	1874873	1612533	46.64%	6.911%
5	6.734	787	790	794	rBV	792972	732565	21.19%	3.140%
6	6.893	813	817	821	rBV	2542038	2422362	70.07%	10.382%
7	7.304	881	887	890	rBV	1858704	2089736	60.45%	8.956%
8	8.022	1004	1009	1012	rBV	941072	962799	27.85%	4.126%
9	9.098	1186	1192	1195	rBV	3295987	3457048	100.00%	14.816%
10	9.739	1298	1301	1303	rBV	104918	102495	2.96%	0.439%
11	9.775	1303	1307	1311	rVB2	1047499	1066527	30.85%	4.571%
12	10.557	1434	1440	1443	rBV	1336631	1187825	34.36%	5.091%
13	10.639	1450	1454	1456	rBV	127334	118207	3.42%	0.507%
14	11.145	1534	1540	1548	rVB2	86061	106775	3.09%	0.458%
15	11.251	1553	1558	1562	rBV	1109483	1000427	28.94%	4.288%
16	11.392	1579	1582	1585	rVB	90724	71318	2.06%	0.306%
17	11.551	1605	1609	1612	rBV4	24394	40206	1.16%	0.172%
18	11.828	1651	1656	1665	rBV2	310976	308283	8.92%	1.321%
19	12.210	1718	1721	1724	rBV	65178	64697	1.87%	0.277%
20	12.351	1742	1745	1748	rBV2	47799	56868	1.64%	0.244%
21	12.386	1748	1751	1754	rVV3	24882	37442	1.08%	0.160%
22	12.492	1766	1769	1772	rBV2	50959	80673	2.33%	0.346%
23	12.622	1788	1791	1795	rBV4	48776	64473	1.86%	0.276%
24	12.698	1801	1804	1806	rBV2	45276	45197	1.31%	0.194%
25	12.722	1806	1808	1810	rBV2	56578	49949	1.44%	0.214%
26	12.839	1823	1828	1832	rBV	2672642	2897646	83.82%	12.419%
27	12.874	1832	1834	1841	rVB	269921	271751	7.86%	1.165%
28	13.069	1865	1867	1870	rBV3	67164	74382	2.15%	0.319%
29	13.198	1887	1889	1893	rBV	89282	98672	2.85%	0.423%
30	13.533	1943	1946	1955	rVB3	135674	266245	7.70%	1.141%
31	13.804	1990	1992	1996	rVB	142390	122184	3.53%	0.524%
32	13.857	1998	2001	2002	rVV2	128409	158422	4.58%	0.679%
33	13.886	2002	2006	2009	rVB	821975	824184	23.84%	3.532%
34	14.163	2051	2053	2061	rVB2	150585	218936	6.33%	0.938%

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Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
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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

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35	15.304	2243	2247	2252	rBV	478766	531993	15.39%	2.280%
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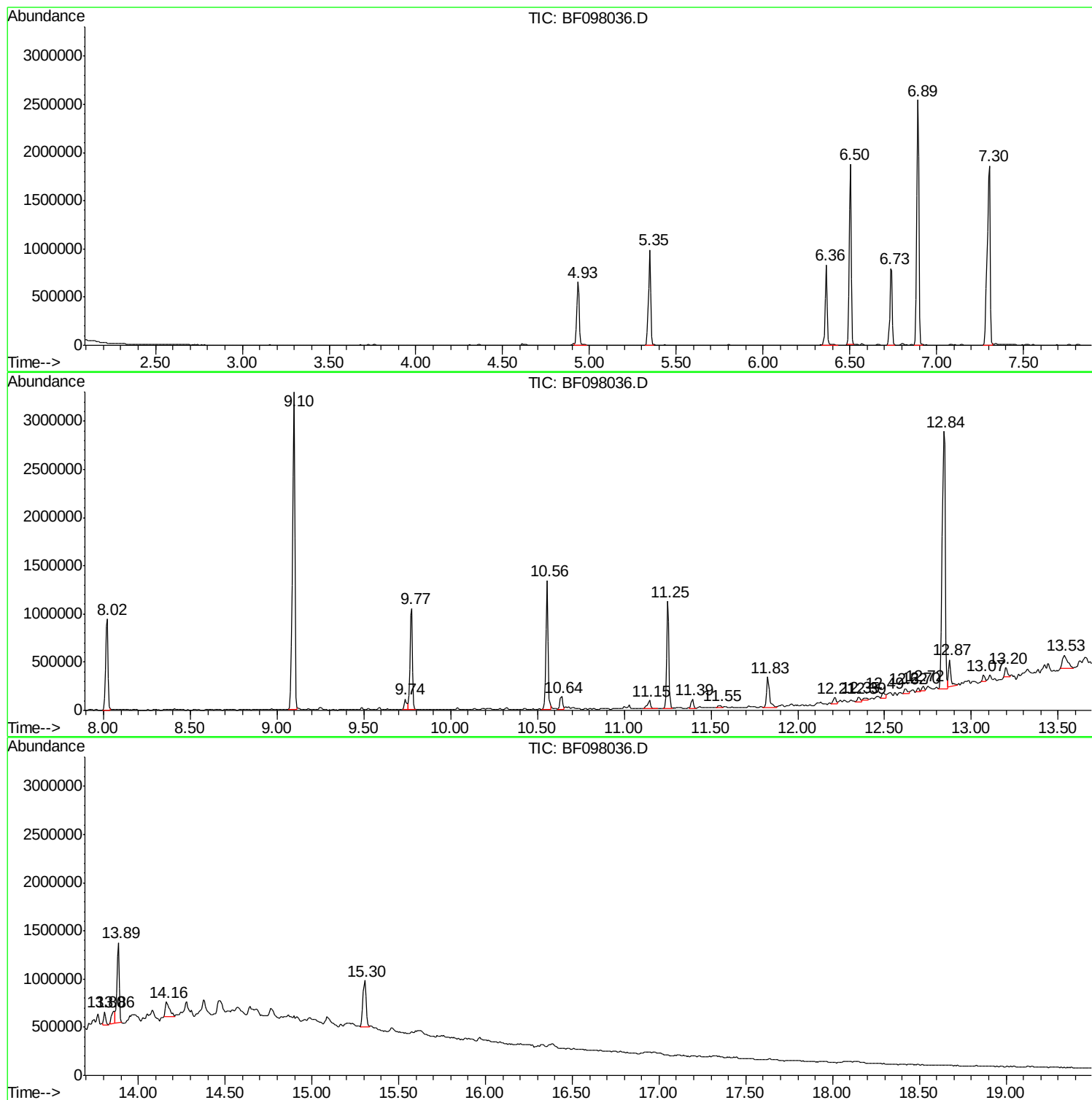
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF081517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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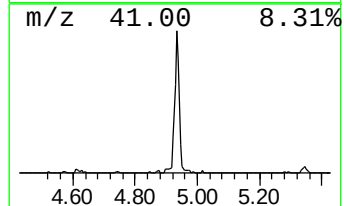
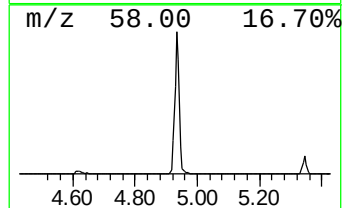
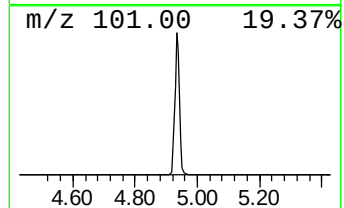
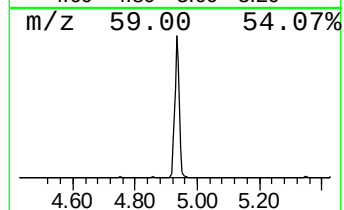
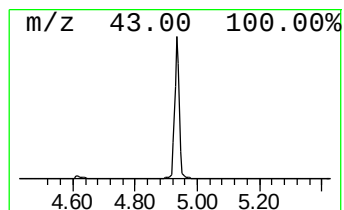
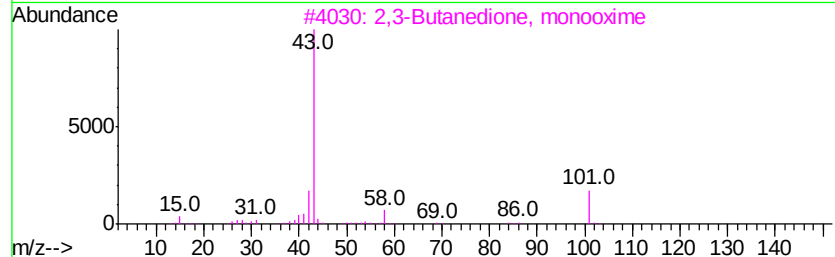
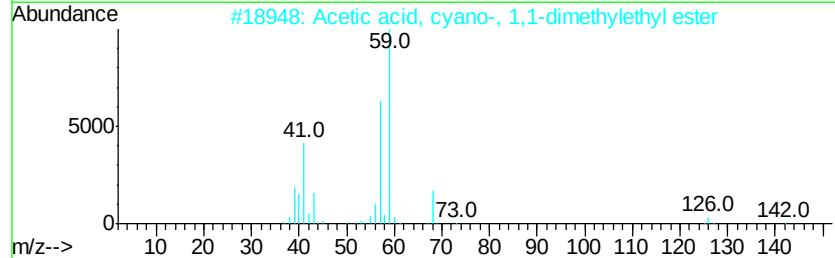
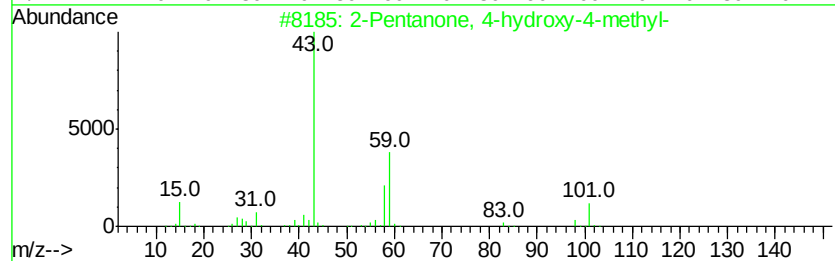
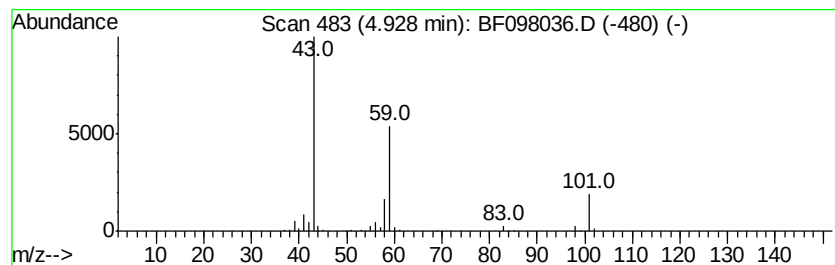
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.93	18.74 ng	686288	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	50
2		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	17
3		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	12
4		(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
5		Acetone	58	C3H6O	000067-64-1	9



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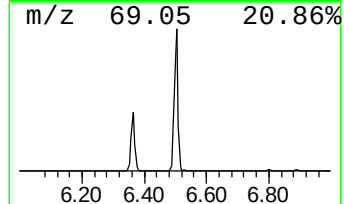
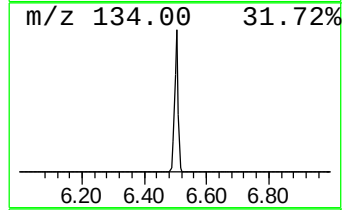
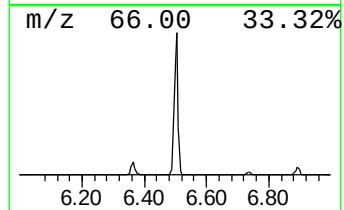
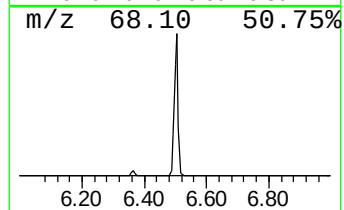
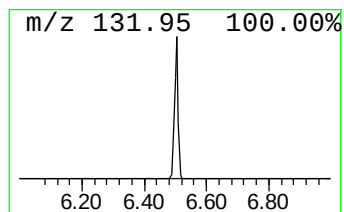
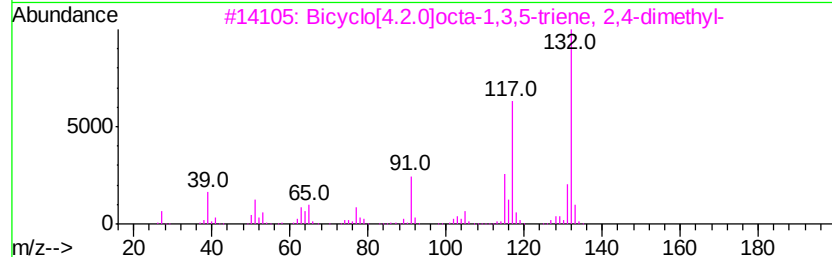
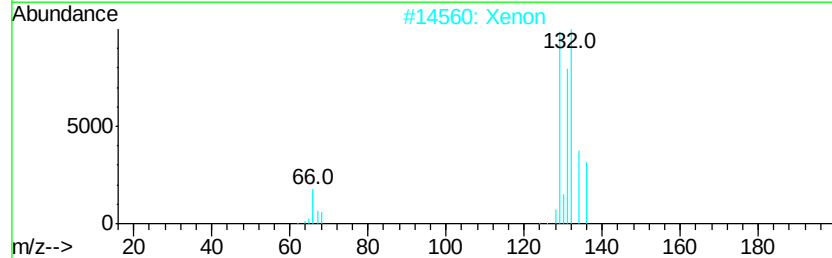
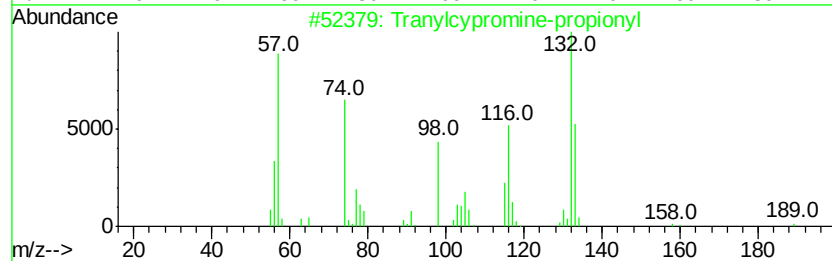
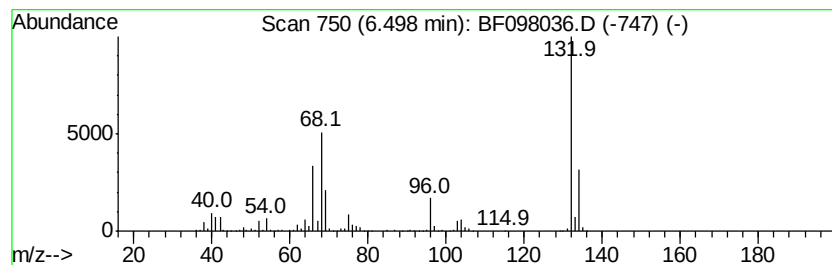
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.50 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.50	44.02 ng	1612530	1,4-Dichlorobenzene-d4	6.74

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
2		Xenon	132	Xe	007440-63-3	9
3		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9



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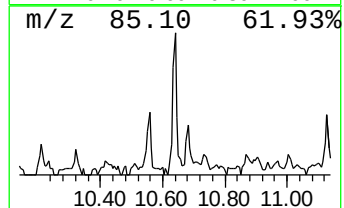
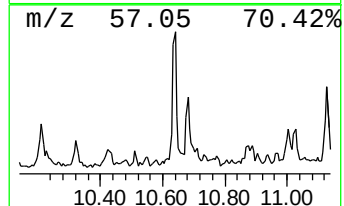
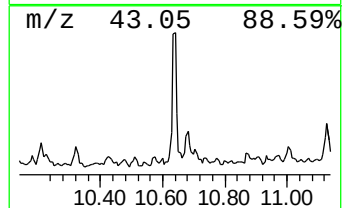
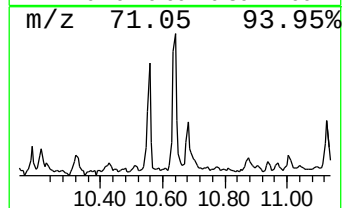
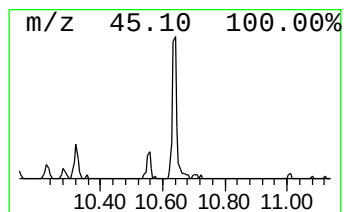
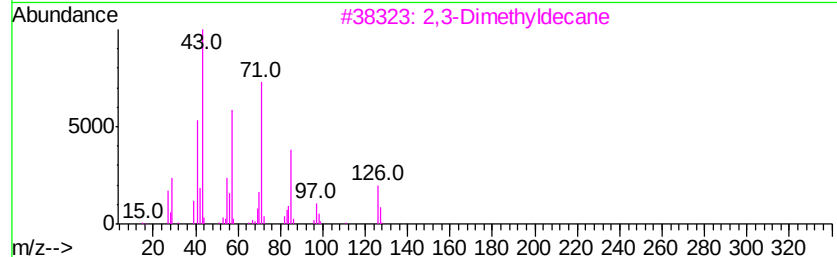
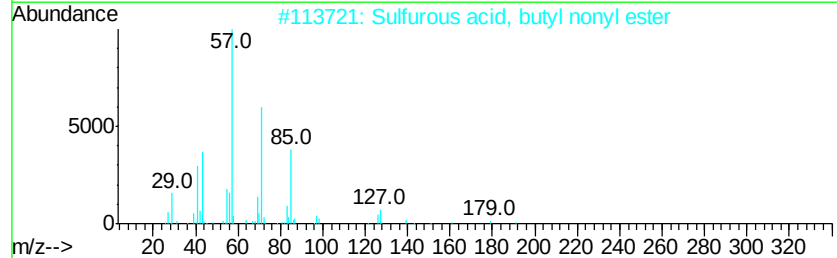
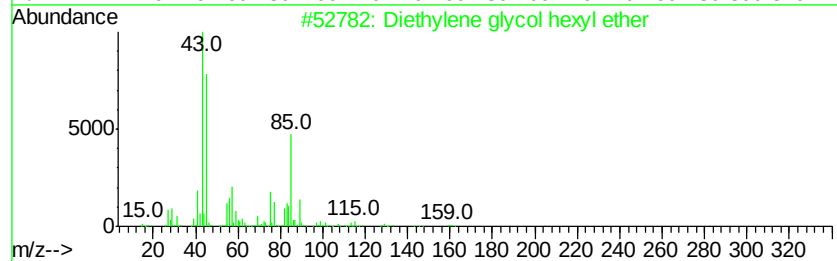
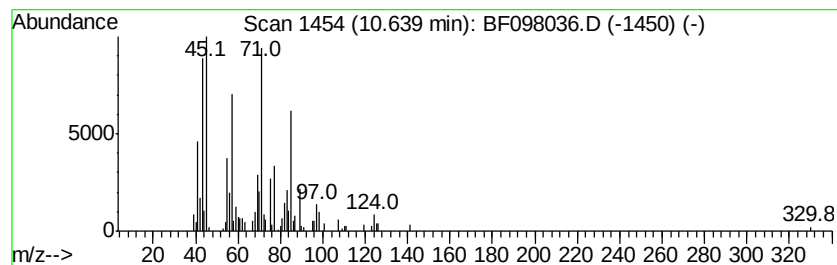
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown10.64 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.64	2.36 ng	118207	Phenanthrene-d10	11.25

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Diethylene glycol hexyl ether	190	C10H22O3	000112-59-4	38
2		Sulfurous acid, butyl nonyl ester	264	C13H28O3S	1000309-17-6	38
3		2,3-Dimethyldecane	170	C12H26	017312-44-6	35
4		Dodecane, 2,6,10-trimethyl-	212	C15H32	003891-98-3	35
5		Hexadecane	226	C16H34	000544-76-3	35



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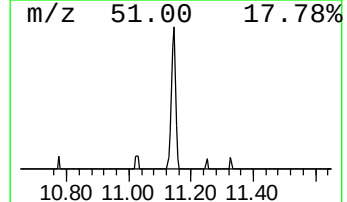
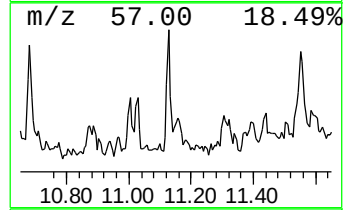
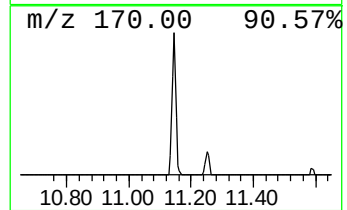
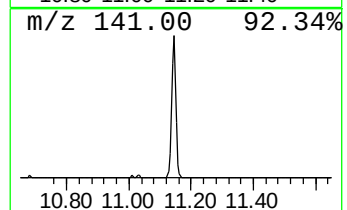
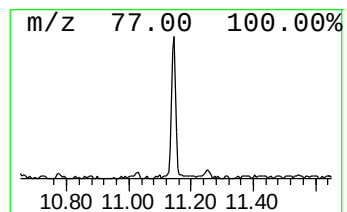
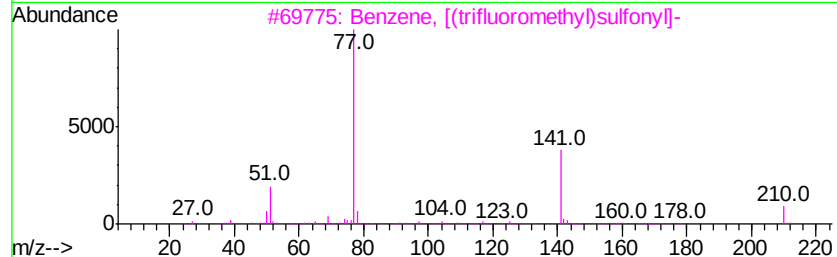
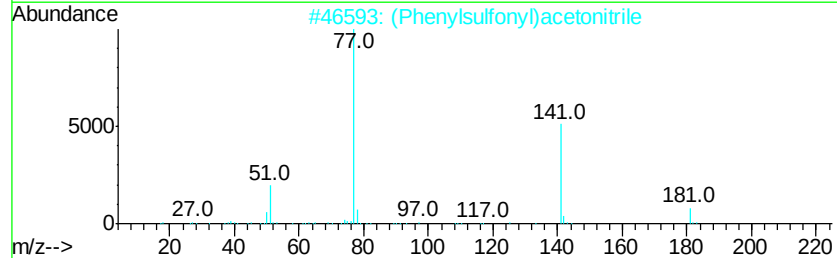
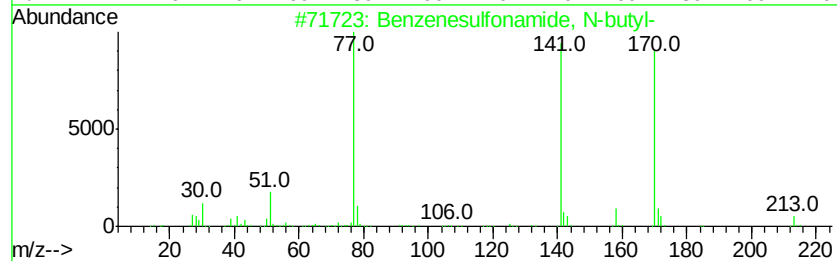
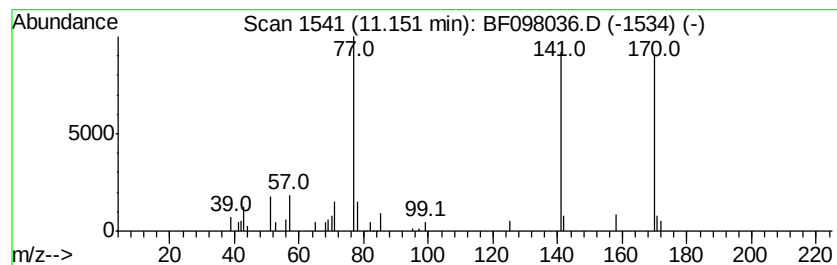
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Benzenesulfonamide, N-butyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.15	2.13 ng	106775	Phenanthrene-d10	11.25

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzenesulfonamide, N-butyl-	213	C10H15N02S	003622-84-2	91
2		(Phenylsulfonyl)acetonitrile	181	C8H7N02S	007605-28-9	59
3		Benzene, [(trifluoromethyl)sulfo...	210	C7H5F3O2S	000426-58-4	59
4		N-Benzenesulfonyloxy-2,2-bis(tri...	335	C10H7F6N03S	055734-41-3	45
5		Benzenesulfonyl isocyanate	183	C7H5N03S	002845-62-7	45



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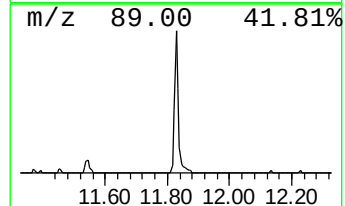
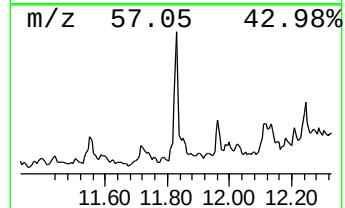
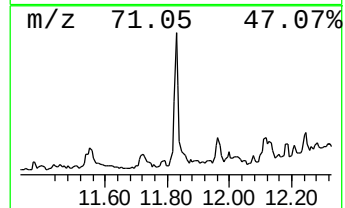
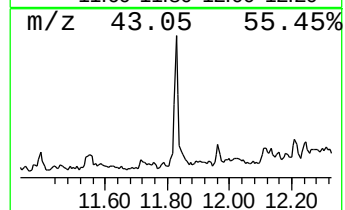
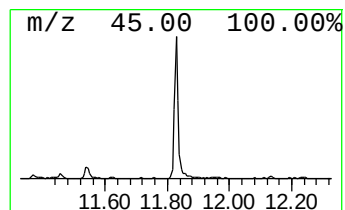
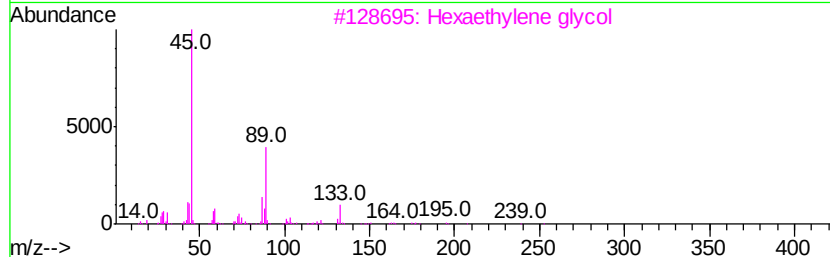
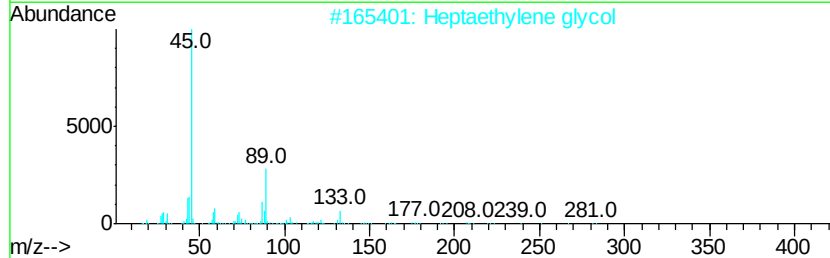
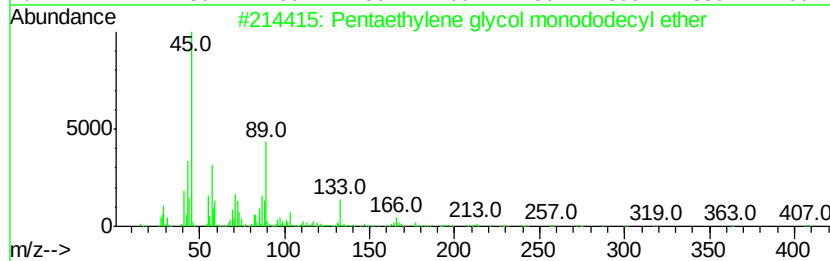
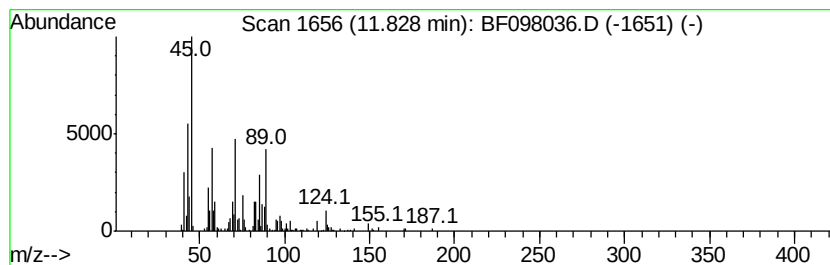
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 6 Pentaethylene glycol monodo... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.83	6.16 ng	308283	Phenanthrene-d10	11.25

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Pentaethylene glycol monododecyl...	406	C22H46O6	003055-95-6	58
2		Heptaethylene glycol	326	C14H30O8	005617-32-3	52
3		Hexaethylene glycol	282	C12H26O7	002615-15-8	52
4		Pentaethylene glycol	238	C10H22O6	004792-15-8	52
5		Tetraethylene glycol	194	C8H18O5	000112-60-7	50



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ClientSampled :
JPS-W1

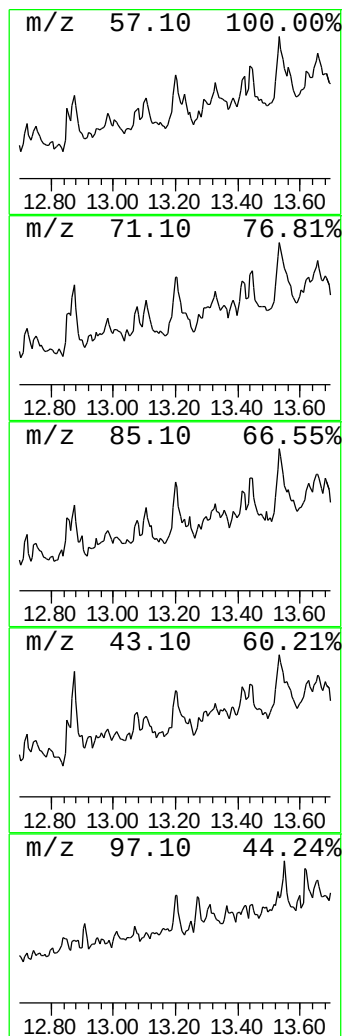
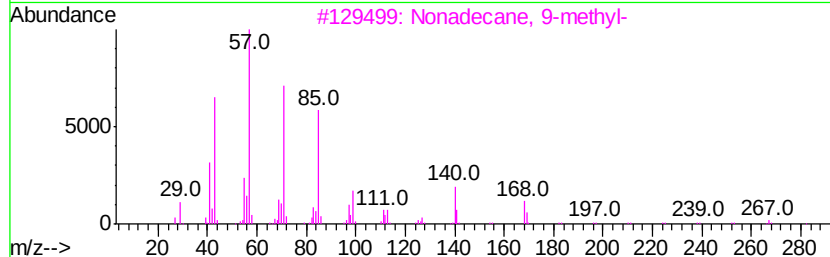
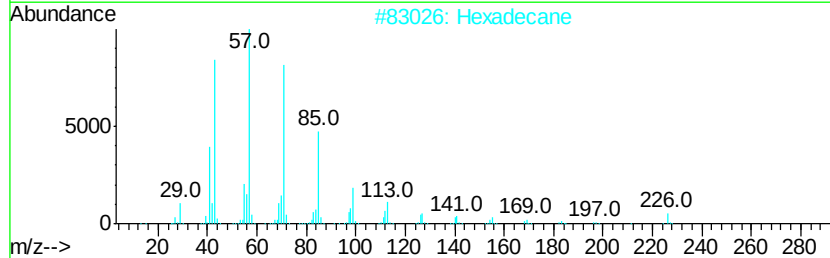
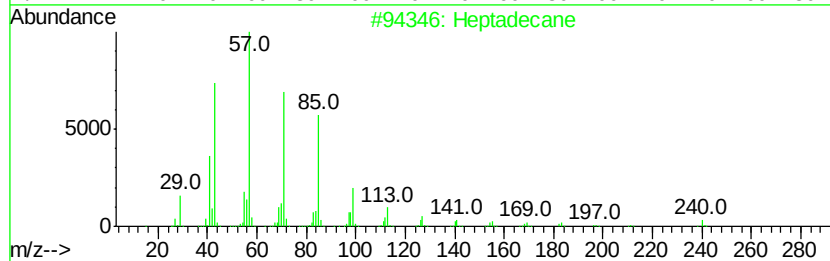
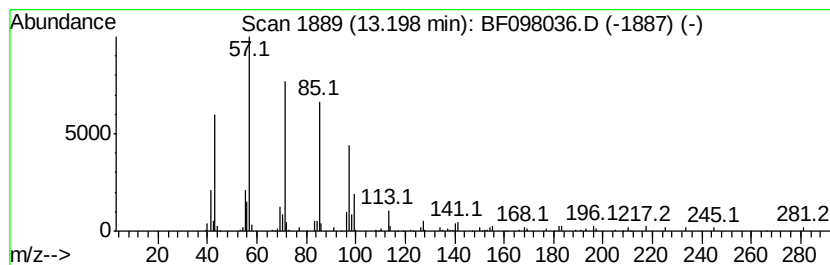
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF081517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Heptadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.20	2.39 ng	98672	Chrysene-d12	13.89

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane		240	C17H36	000629-78-7	64
2	Hexadecane		226	C16H34	000544-76-3	64
3	Nonadecane, 9-methyl-		282	C20H42	013287-24-6	59
4	Decane, 2,3,5-trimethyl-		184	C13H28	062238-11-3	53
5	Tridecane, 7-hexyl-		268	C19H40	007225-66-3	53



Data Path : Z:\HPCHEM1\BNA F\DATA\BF082517\
Data File : BF098036.D
Acq On : 25 Aug 2017 17:56
Operator : SJ/JU
Sample : I4974-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

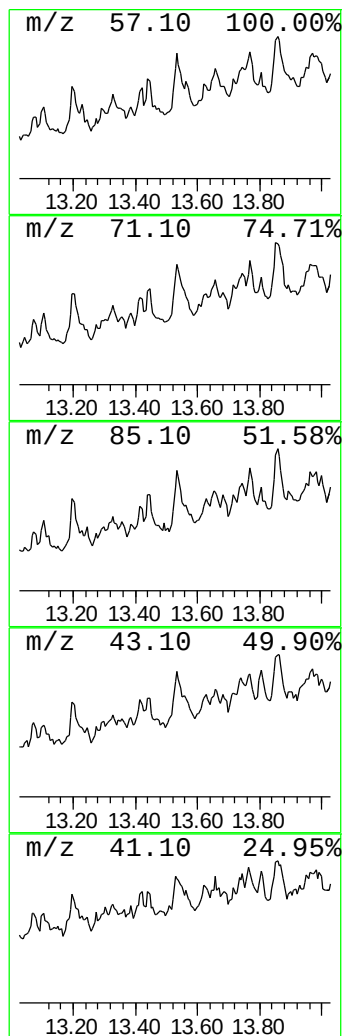
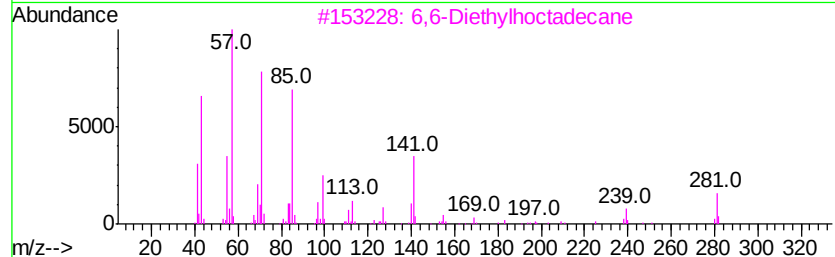
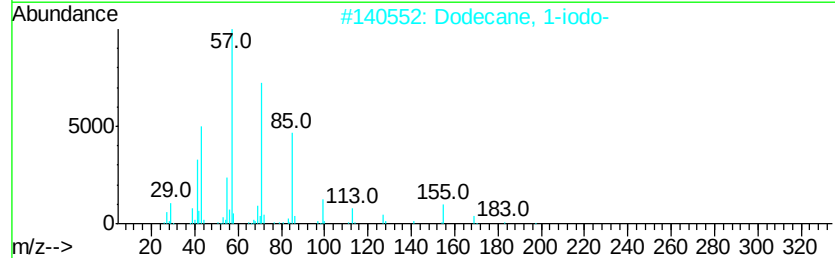
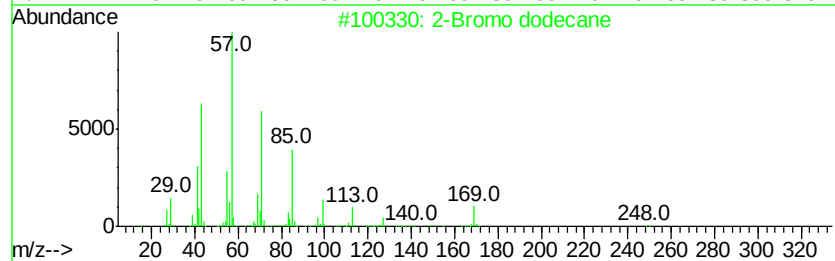
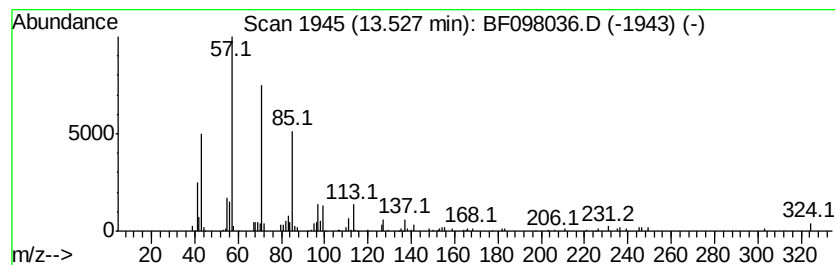
Instrument :
BNA_F
ClientSampleId :
JPS-W1

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF081517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 2-Bromo dodecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.		
13.53	6.46 ng	266245	Chrysene-d12	13.89		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Bromo dodecane	248	C12H25Br	013187-99-0	86	
2	Dodecane, 1-iodo-	296	C12H25I	004292-19-7	80	
3	6,6-Diethylhooctadecane	310	C22H46	1000360-41-8	78	
4	Undecane, 5-ethyl-5-propyl-	226	C16H34	002755-07-9	72	
5	Sulfurous acid, butyl decyl ester	278	C14H30O3S	1000309-17-7	59	



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF082517\
Data File : BF098036.D
Acq On : 25 Aug 2017 17:56
Operator : SJ/JU
Sample : I4974-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

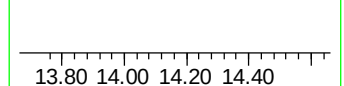
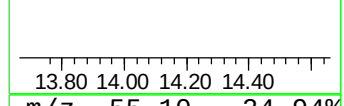
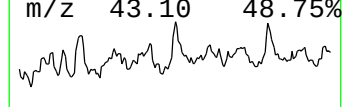
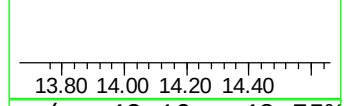
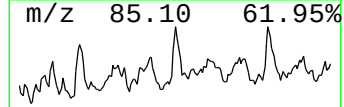
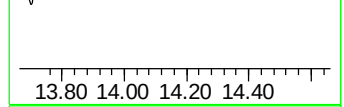
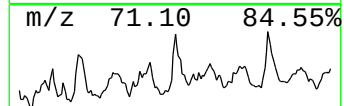
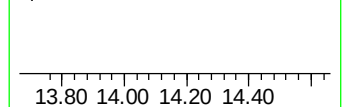
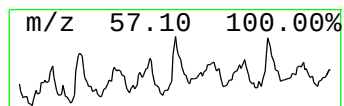
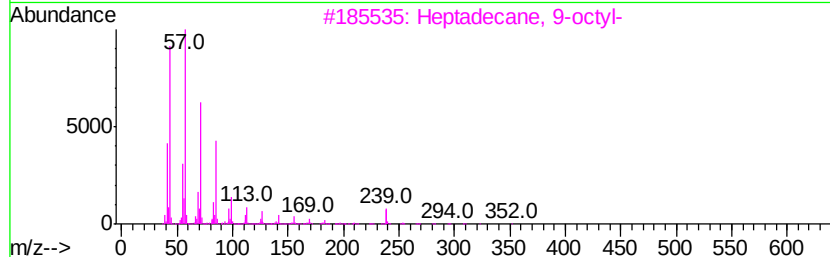
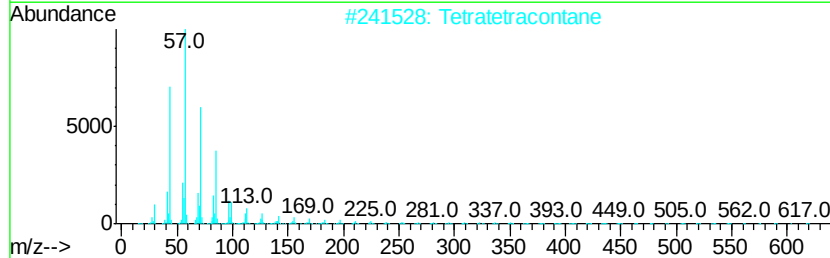
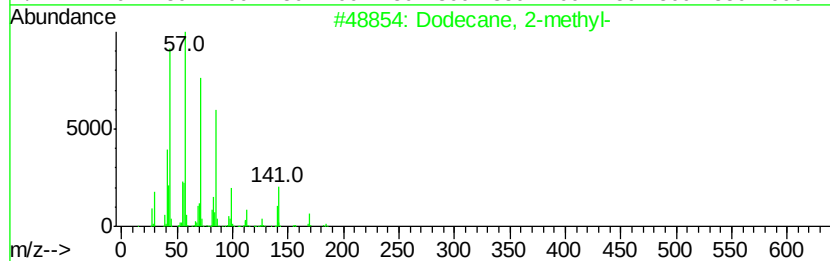
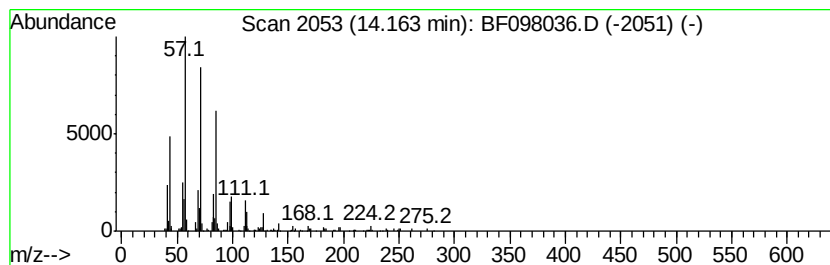
Instrument :
BNA_F
ClientSampleId :
JPS-W1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Dodecane, 2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.16	5.31 ng	218936	Chrysene-d12	13.89	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecane, 2-methyl-	184	C13H28	001560-97-0	87
2	Tetratetracontane	619	C44H90	007098-22-8	80
3	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	78
4	Hexatriacontane	507	C36H74	000630-06-8	72
5	Octadecane, 1-iodo-	380	C18H37I	000629-93-6	72



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF082517\
Data File : BF098036.D
Acq On : 25 Aug 2017 17:56
Operator : SJ/JU
Sample : I4974-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
JPS-W1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.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...	4.93	18.7	ng	686288	1	6.74	732565	20.0
unknown6.50	6.50	44.0	ng	1612530	1	6.74	732565	20.0
unknown10.64	10.64	2.4	ng	118207	4	11.25	1000430	20.0
Benzenesulfonamid...	11.15	2.1	ng	106775	4	11.25	1000430	20.0
Pentaethylene gly...	11.83	6.2	ng	308283	4	11.25	1000430	20.0
Heptadecane	13.20	2.4	ng	98672	5	13.89	824184	20.0
2-Bromo dodecane	13.53	6.5	ng	266245	5	13.89	824184	20.0
Dodecane, 2-methyl-	14.16	5.3	ng	218936	5	13.89	824184	20.0