

Data Path : Z:\HPCHEM1\BNA F\DATA\BF041218\
 Data File : BF104462.D
 Acq On : 12 Apr 2018 20:16
 Operator : JU/SJ
 Sample : J2310-05
 Misc :
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 P004-S004-0001-01

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:\HPCHEM1\BNA_F\METHODS\8270-BF040618.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	5.022	494	499	505	rVB	92835	118161	4.44%	0.521%
2	5.422	562	567	570	rBV	2411878	2372011	89.12%	10.468%
3	6.445	735	741	751	rVB	2380597	2411486	90.60%	10.642%
4	6.581	759	764	767	rBV	2680476	2463988	92.57%	10.874%
5	6.810	799	803	806	rBV	923694	703098	26.42%	3.103%
6	6.969	825	830	833	rBV	2136410	1891536	71.06%	8.348%
7	7.375	894	899	902	rBV	1648576	1457975	54.78%	6.434%
8	8.092	1017	1021	1024	rBV	1125670	880413	33.08%	3.885%
9	9.169	1200	1204	1207	rBV	2966158	2661706	100.00%	11.747%
10	9.563	1267	1271	1274	rBV	176113	141082	5.30%	0.623%
11	9.775	1302	1307	1311	rVB	67522	56845	2.14%	0.251%
12	9.851	1316	1320	1324	rBV	1004869	841846	31.63%	3.715%
13	10.275	1390	1392	1395	rVB	91918	70083	2.63%	0.309%
14	10.492	1425	1429	1432	rBV	26572	31594	1.19%	0.139%
15	10.639	1450	1454	1458	rBV	1553990	1330760	50.00%	5.873%
16	10.751	1470	1473	1482	rBV	127194	122685	4.61%	0.541%
17	11.198	1546	1549	1552	rBV	83413	65473	2.46%	0.289%
18	11.280	1561	1563	1568	rBV4	28881	30319	1.14%	0.134%
19	11.339	1569	1573	1576	rVV	902359	728681	27.38%	3.216%
20	11.392	1579	1582	1588	rVB3	28005	30031	1.13%	0.133%
21	11.504	1598	1601	1606	rVB	46839	39581	1.49%	0.175%
22	11.557	1606	1610	1617	rBV7	24329	38069	1.43%	0.168%
23	11.869	1659	1663	1666	rBV	107040	105514	3.96%	0.466%
24	12.480	1764	1767	1770	rVB	44303	36398	1.37%	0.161%
25	12.927	1839	1843	1847	rBV	2134059	2101686	78.96%	9.275%
26	13.821	1992	1995	2000	rVB	325177	301162	11.31%	1.329%
27	13.963	2016	2019	2020	rBV	167740	128293	4.82%	0.566%
28	13.986	2020	2023	2027	rVB	712189	638941	24.00%	2.820%
29	14.457	2101	2103	2106	rBV	79040	77700	2.92%	0.343%
30	14.745	2149	2152	2160	rVB	245799	288054	10.82%	1.271%
31	15.451	2268	2272	2280	rVB	374780	494153	18.57%	2.181%

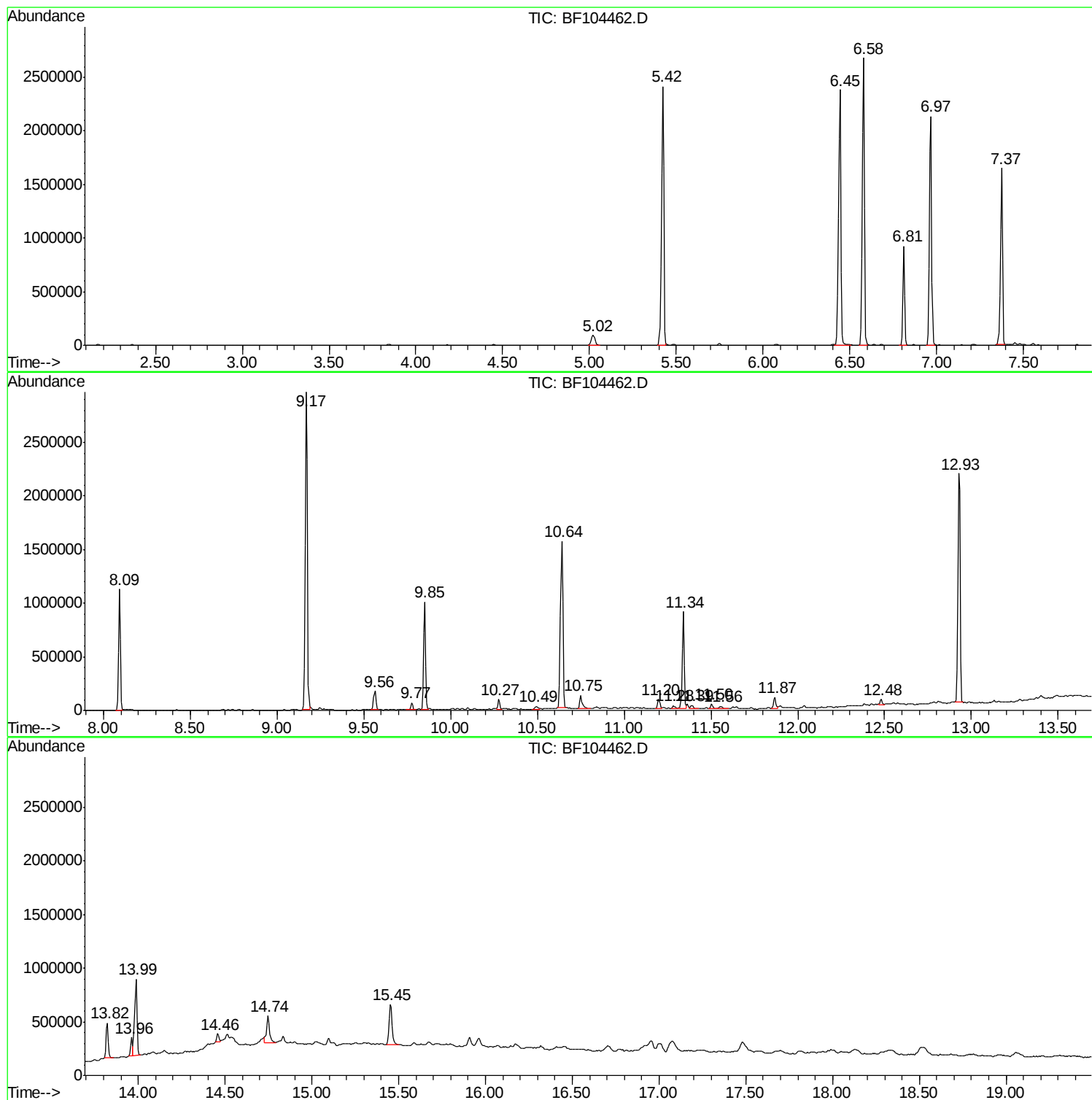
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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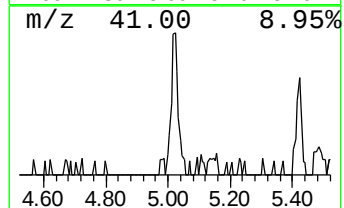
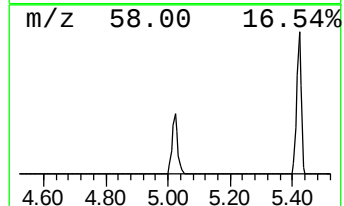
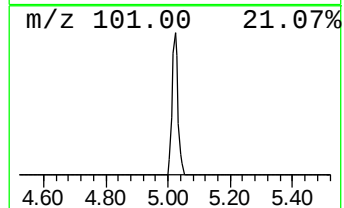
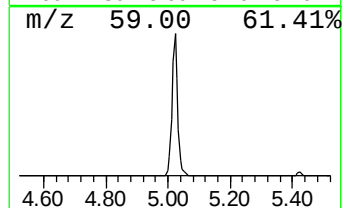
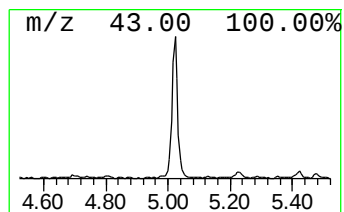
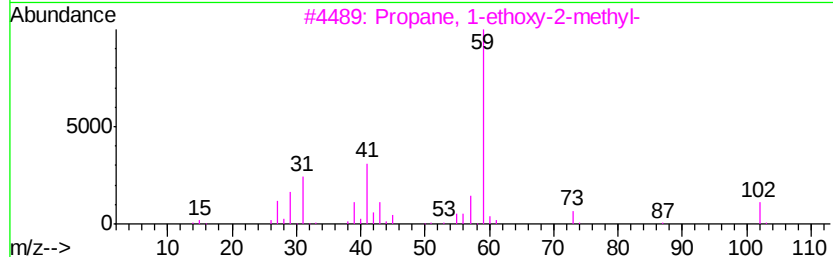
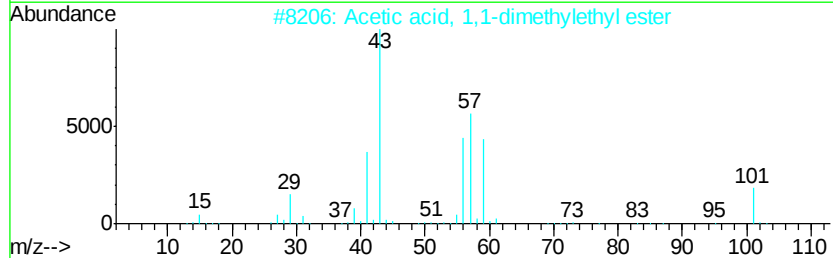
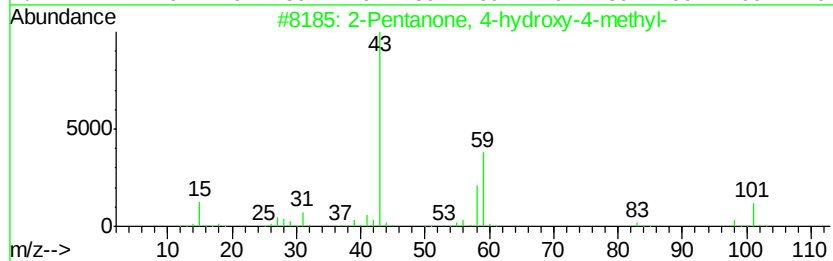
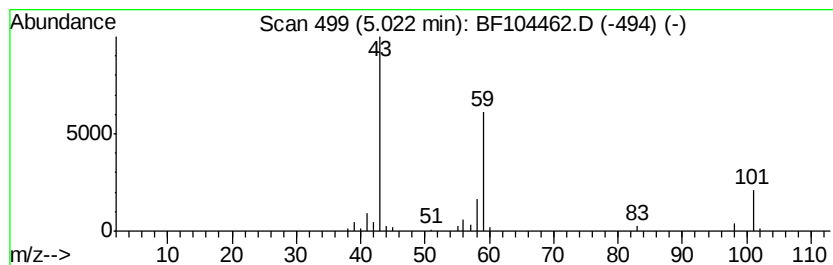
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Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.02	3.36 ng	118161	1,4-Dichlorobenzene-d4	6.81

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2		000123-42-2	56
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2		000540-88-5	38
3	Propane, 1-ethoxy-2-methyl-	102	C6H14O		000627-02-1	35
4	2,3-Butanedione, monooxime	101	C4H7NO2		000057-71-6	25
5	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O		017348-59-3	23



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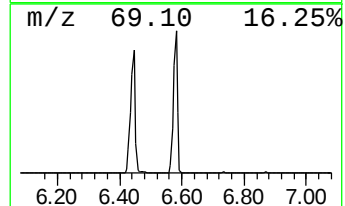
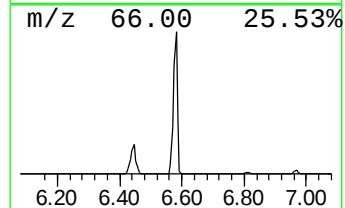
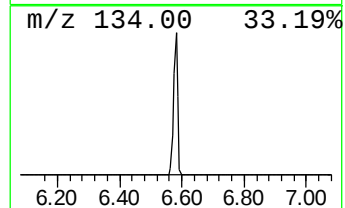
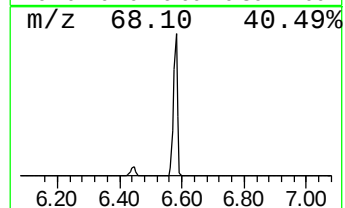
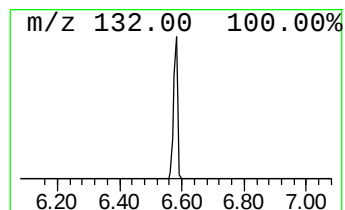
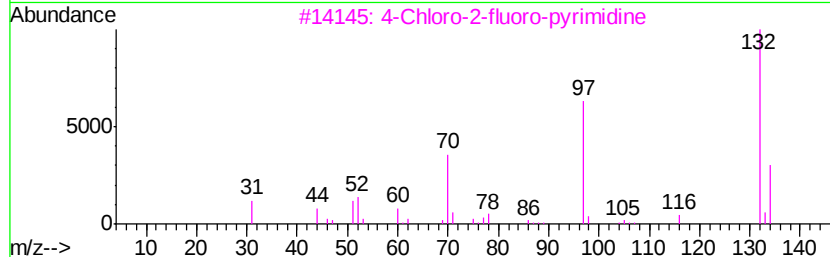
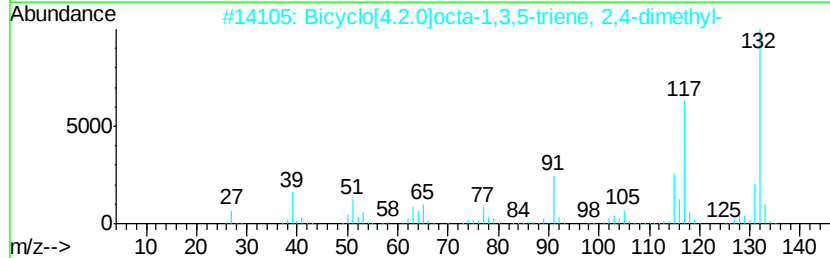
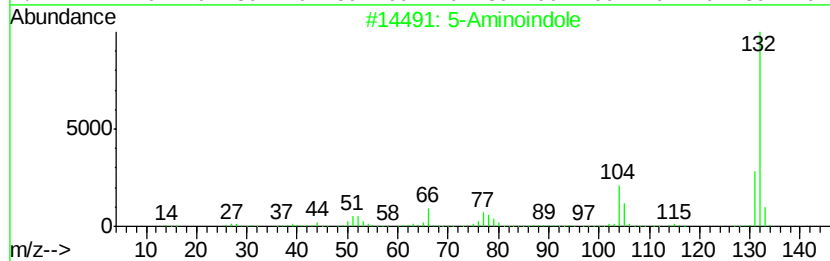
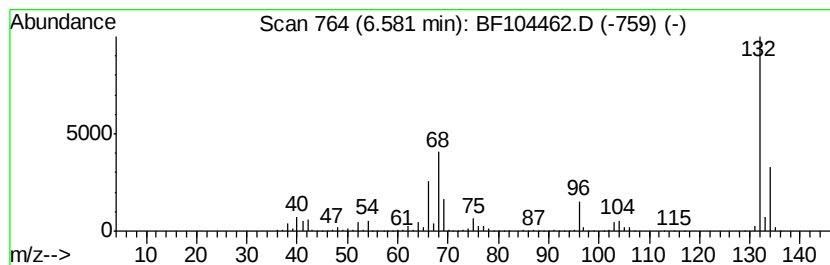
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Peak Number 2 unknown6.58 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.58	70.09 ng	2463990	1,4-Dichlorobenzene-d4	6.81

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	5-Aminoindole	132	C8H8N2	005192-03-0	12
2		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
3		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
4		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	9



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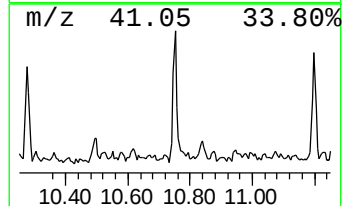
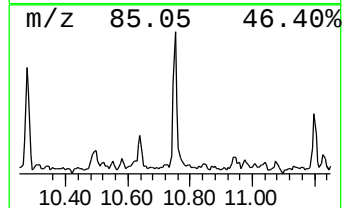
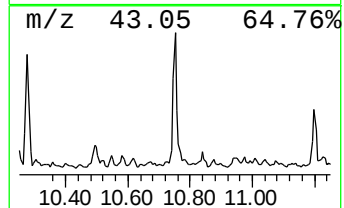
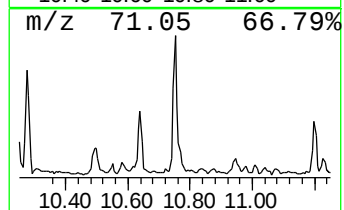
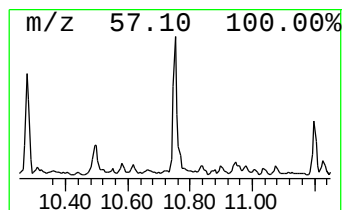
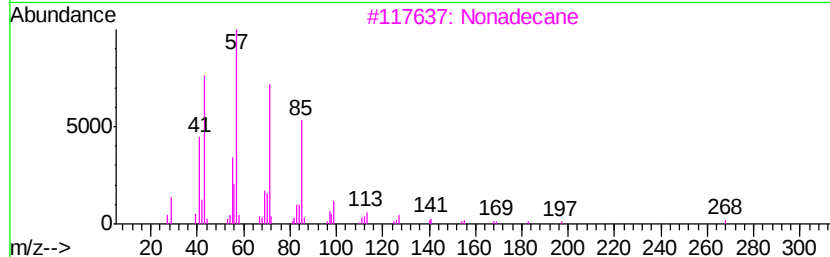
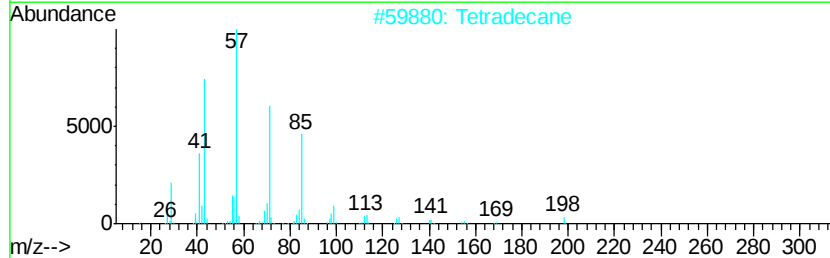
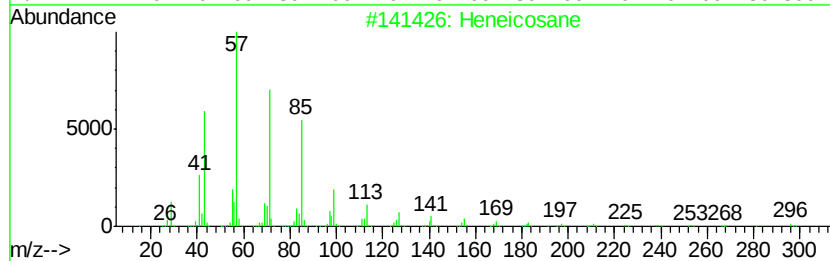
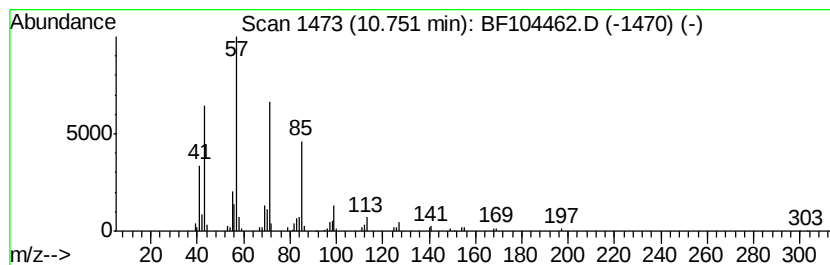
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TIC Integration Parameters: LSCINT.P

Peak Number 4 Heneicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.75	3.37 ng	122685	Phenanthrene-d10	11.34

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane		296	C21H44	000629-94-7	91
2	Tetradecane		198	C14H30	000629-59-4	91
3	Nonadecane		268	C19H40	000629-92-5	90
4	Hexadecane		226	C16H34	000544-76-3	90
5	Heptadecane		240	C17H36	000629-78-7	87



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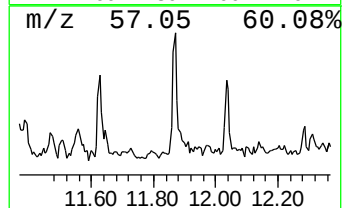
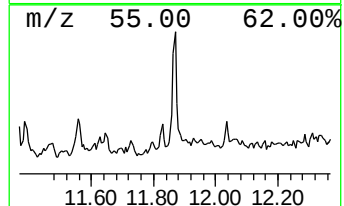
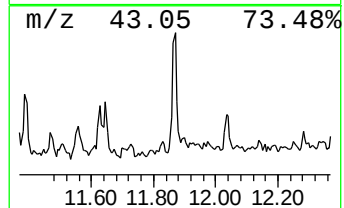
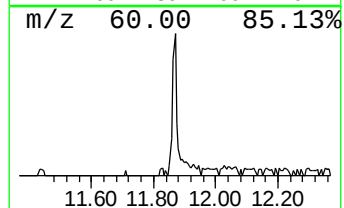
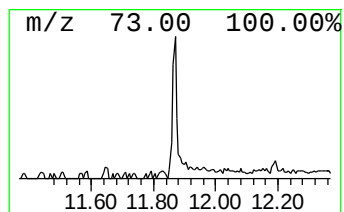
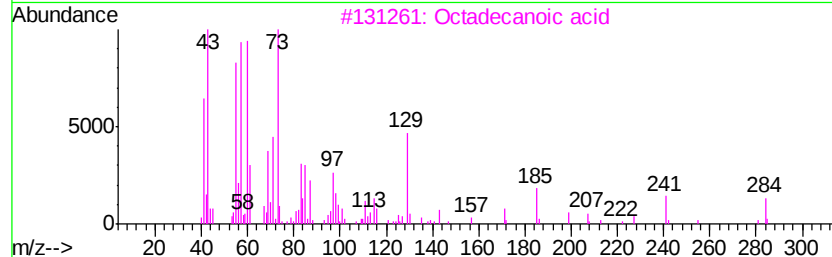
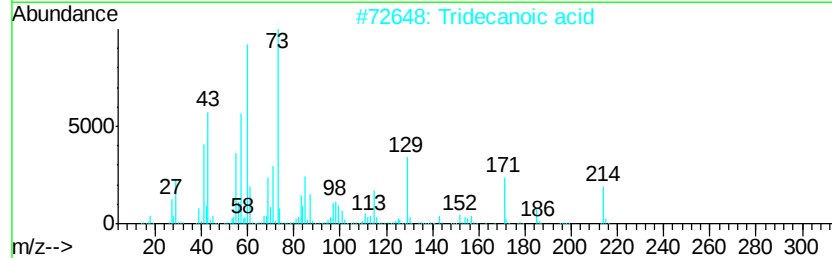
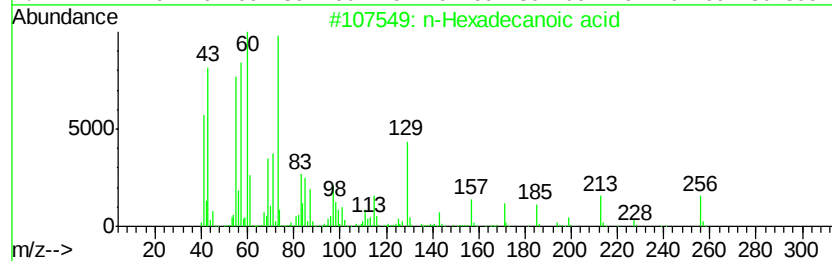
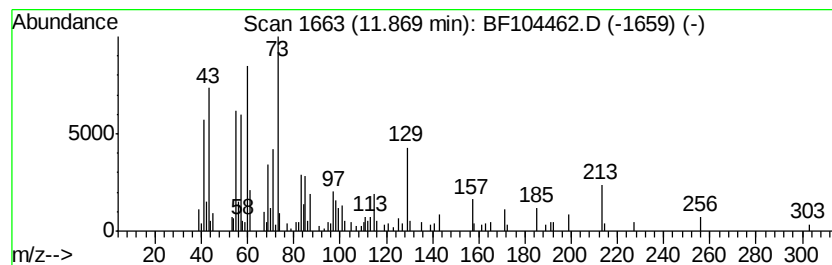
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Peak Number 5 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD		R.T.
11.87	2.90 ng	105514	Phenanthrene-d10		11.34
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	93
3	Octadecanoic acid	284	C18H36O2	000057-11-4	87
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	83
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	83



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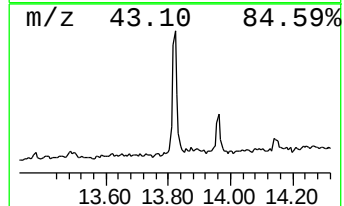
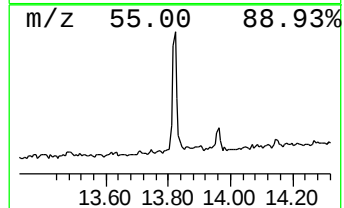
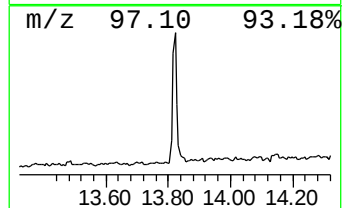
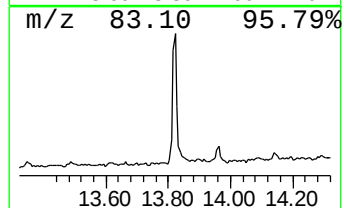
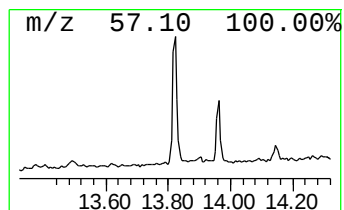
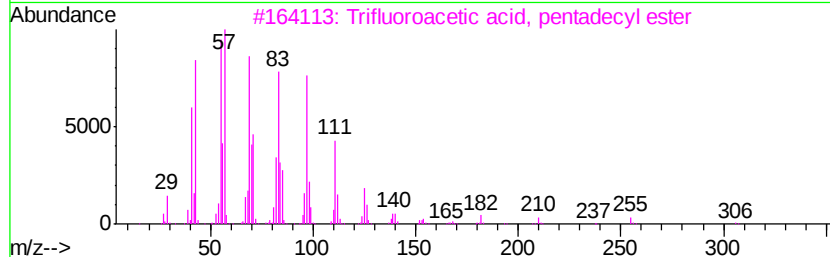
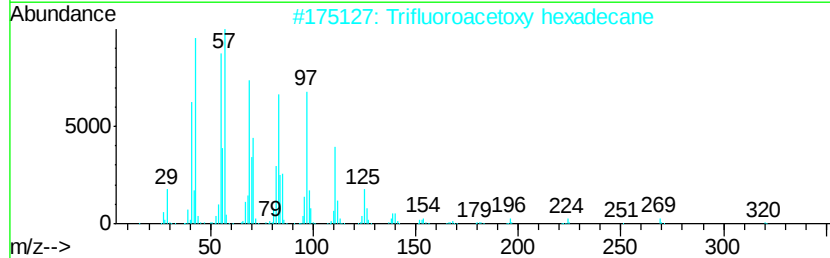
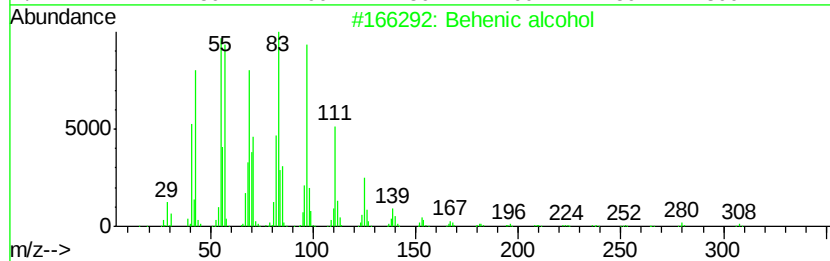
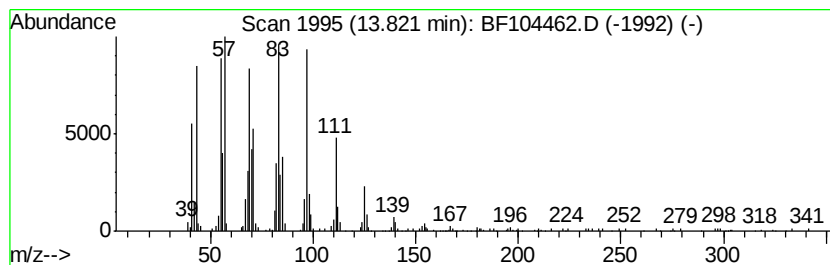
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Peak Number 6 Behenic alcohol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.82	9.43 ng	301162	Chrysene-d12	13.99

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Behenic alcohol	326	C22H46O	000661-19-8	95
2		Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
3		Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	94
4		Heptafluorobutyric acid, penta...	424	C19H31F7O2	959261-23-5	93
5		Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	93



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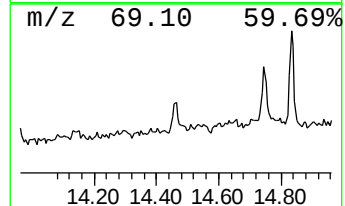
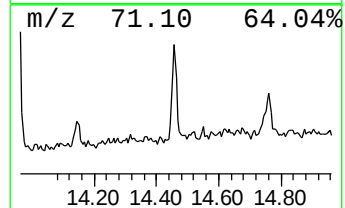
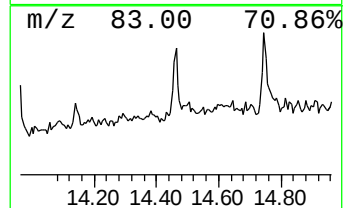
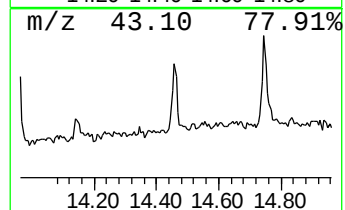
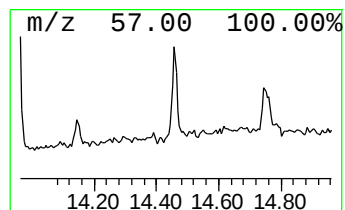
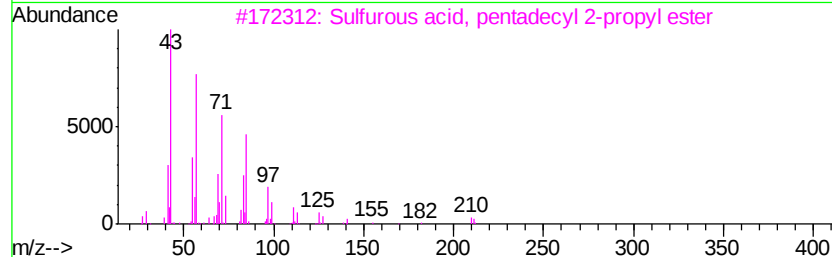
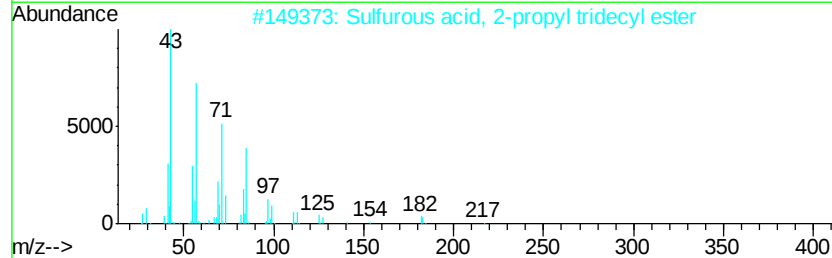
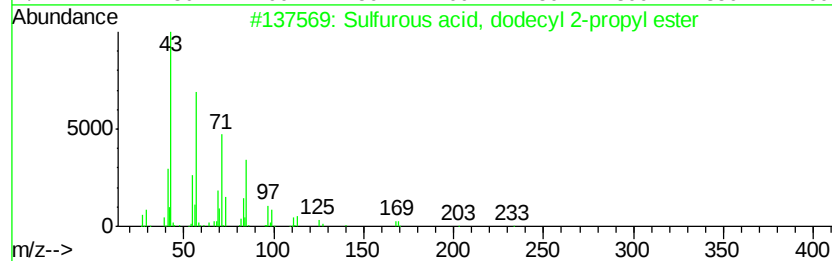
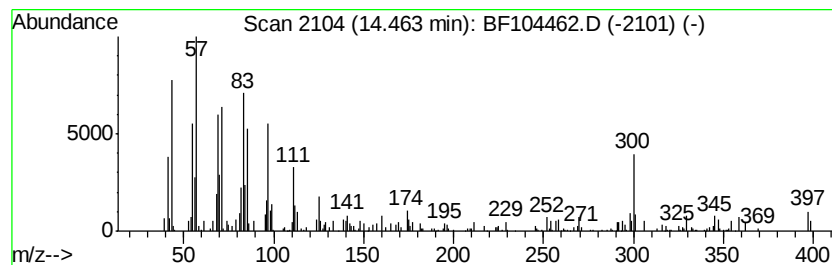
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Sulfurous acid, dodecyl 2-p... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.46	2.43 ng	77700	Chrysene-d12	13.99

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Sulfurous acid, dodecyl 2-propyl...	292	C15H32O3S	1000309-12-3	68
2		Sulfurous acid, 2-propyl tridecyl...	306	C16H34O3S	1000309-12-4	68
3		Sulfurous acid, pentadecyl 2-pro...	334	C18H38O3S	1000309-12-6	64
4		Hexacosane	366	C26H54	000630-01-3	62
5		Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	58



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF041218\
Data File : BF104462.D
Acq On : 12 Apr 2018 20:16
Operator : JU/SJ
Sample : J2310-05
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P004-S004-0001-01

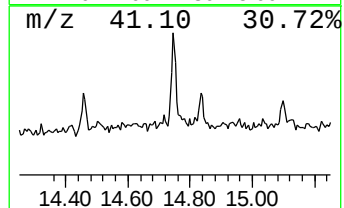
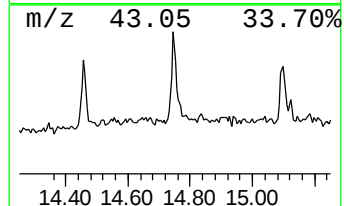
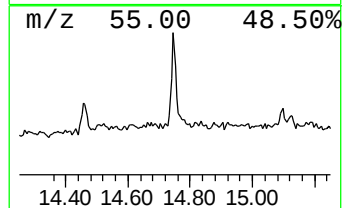
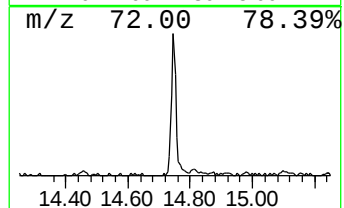
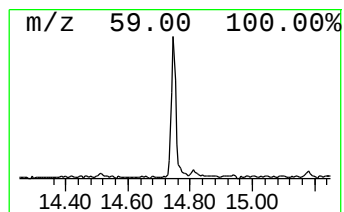
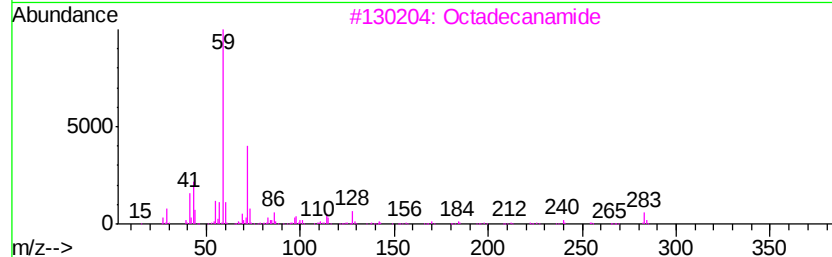
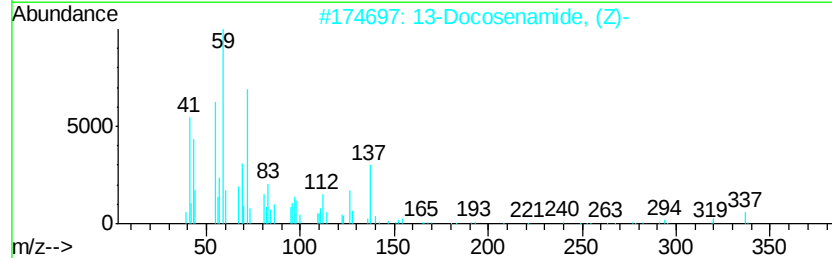
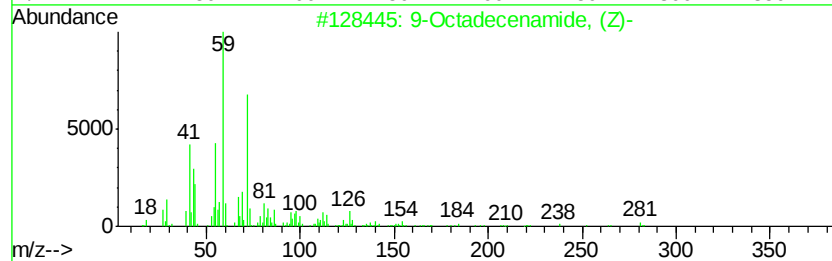
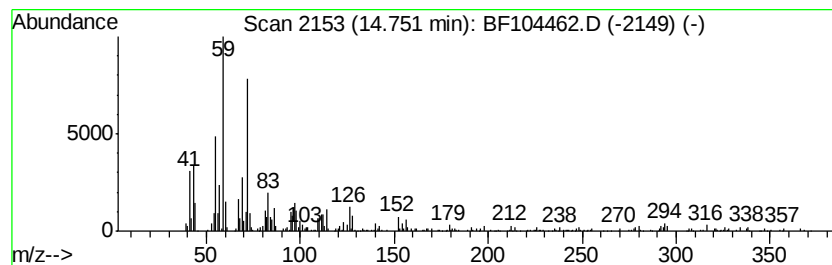
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 9-Octadecenamide, (Z)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.75	11.66 ng	288054	Perylene-d12	15.45

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	83
2		13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	59
3		Octadecanamide	283	C18H37NO	000124-26-5	47
4		Benzeneethanamine, 2-fluoro-.bet...	229	C11H16FN03	061338-98-5	43
5		Dodecanamide	199	C12H25NO	001120-16-7	38



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF041218\
Data File : BF104462.D
Acq On : 12 Apr 2018 20:16
Operator : JU/SJ
Sample : J2310-05
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P004-S004-0001-01

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.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...	5.02	3.4	ng	118161	1	6.81	703098	20.0
unknown6.58	6.58	70.1	ng	2463990	1	6.81	703098	20.0
Heneicosane	10.75	3.4	ng	122685	4	11.34	728681	20.0
n-Hexadecanoic acid	11.87	2.9	ng	105514	4	11.34	728681	20.0
Behenic alcohol	13.82	9.4	ng	301162	5	13.99	638941	20.0
Sulfurous acid, d...	14.46	2.4	ng	77700	5	13.99	638941	20.0
9-Octadecenamide,...	14.75	11.7	ng	288054	6	15.45	494153	20.0