

Data Path : Z:\HPCHEM1\BNA F\DATA\BF050917\
 Data File : BF095032.D
 Acq On : 9 May 2017 20:39
 Operator : SJ/MA
 Sample : I3014-04
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 RAV-GTMW-3

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-BF050217.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	5.013	519	523	534	rBV	38480	82789	3.38%	0.491%
2	5.654	629	632	658	rBV	372242	833804	34.04%	4.941%
3	7.254	900	904	919	rBV	230176	519900	21.23%	3.081%
4	7.366	919	923	947	rVB	1071795	1613843	65.89%	9.563%
5	7.707	977	981	995	rBV	403792	494401	20.19%	2.929%
6	7.942	1017	1021	1038	rBV	1082974	1370590	55.96%	8.121%
7	8.607	1129	1134	1150	rBV	898261	1210289	49.41%	7.171%
8	9.730	1321	1325	1344	rBV	494611	702970	28.70%	4.165%
9	11.501	1621	1626	1639	rBV	1917470	2449268	100.00%	14.513%
10	12.201	1740	1745	1756	rBV	37015	58745	2.40%	0.348%
11	12.560	1801	1806	1816	rBV2	587249	816369	33.33%	4.837%
12	13.401	1945	1949	1953	rVB2	24817	24779	1.01%	0.147%
13	13.748	2003	2008	2015	rBV	33184	50210	2.05%	0.298%
14	13.854	2021	2026	2041	rBV	919938	1361199	55.58%	8.066%
15	14.177	2076	2081	2091	rBV	22505	36460	1.49%	0.216%
16	14.960	2209	2214	2230	rBV2	540162	775732	31.67%	4.596%
17	15.930	2374	2379	2395	rBV	127166	195168	7.97%	1.156%
18	17.018	2559	2564	2581	rBV	151395	226906	9.26%	1.344%
19	17.289	2604	2610	2621	rBV	1981779	2296728	93.77%	13.609%
20	18.383	2793	2796	2801	rBV2	22433	28030	1.14%	0.166%
21	18.530	2816	2821	2824	rBV2	17530	26087	1.07%	0.155%
22	18.630	2833	2838	2846	rBV	536840	667900	27.27%	3.958%
23	18.718	2851	2853	2859	rVB2	28674	28267	1.15%	0.167%
24	19.153	2920	2927	2930	rBV5	13228	26686	1.09%	0.158%
25	19.242	2939	2942	2948	rBV3	22820	35155	1.44%	0.208%
26	19.324	2950	2956	2960	rBV	60609	79121	3.23%	0.469%
27	19.518	2981	2989	2992	rBV4	32514	68401	2.79%	0.405%
28	19.683	3014	3017	3022	rVB3	25796	35753	1.46%	0.212%
29	19.836	3039	3043	3047	rBV	67232	71222	2.91%	0.422%
30	20.265	3112	3116	3118	rBV	37139	46193	1.89%	0.274%
31	20.294	3118	3121	3133	rVB	409317	550314	22.47%	3.261%
32	20.765	3196	3201	3207	rVB	41044	58845	2.40%	0.349%
33	21.318	3291	3295	3303	rVB5	16565	34552	1.41%	0.205%

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Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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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

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

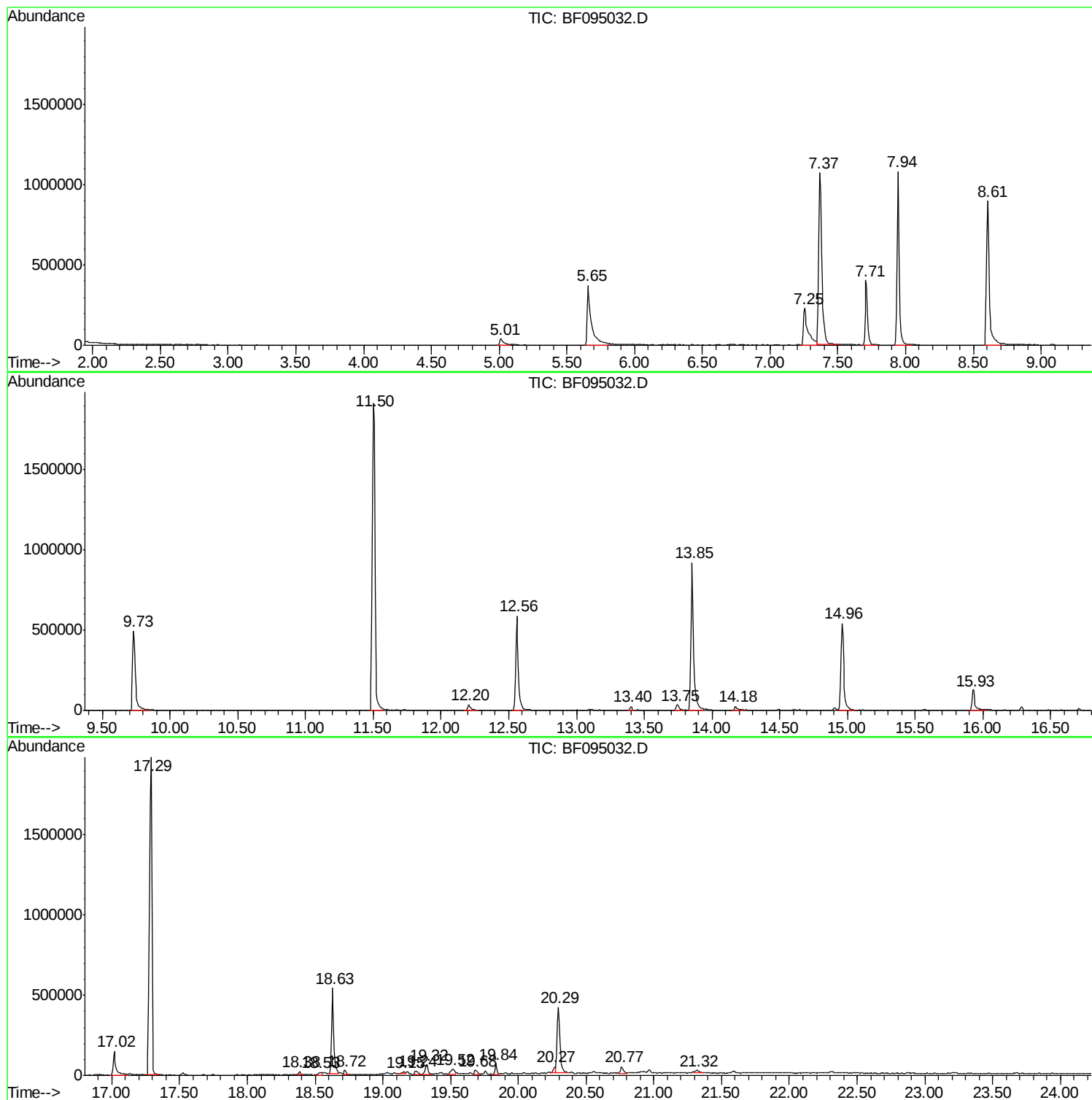
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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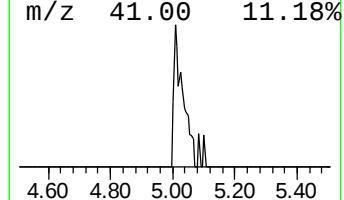
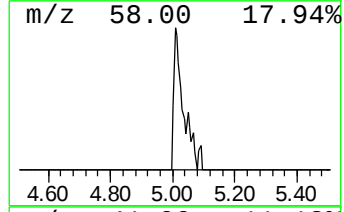
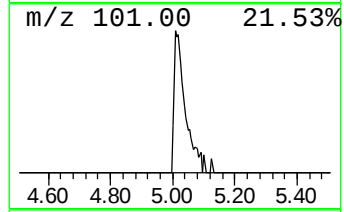
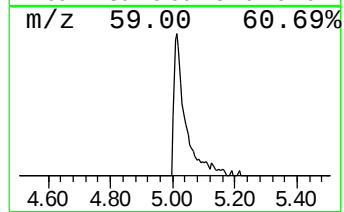
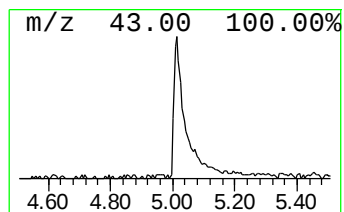
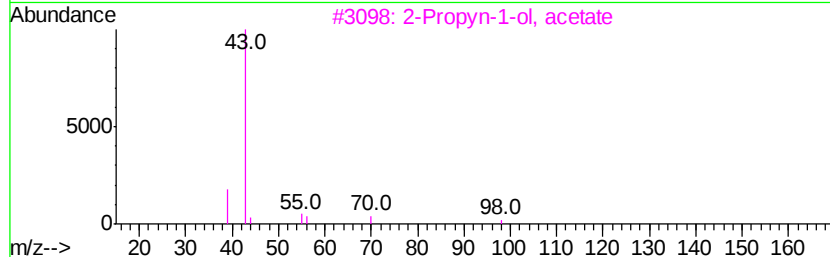
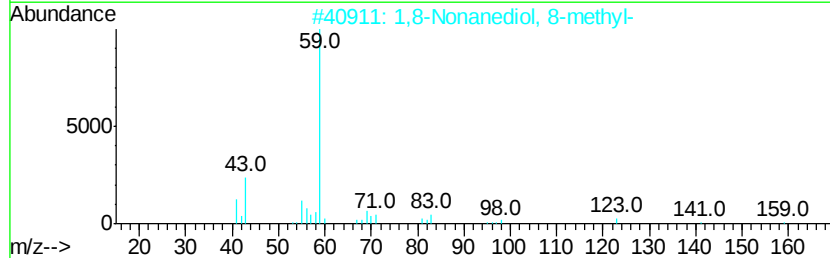
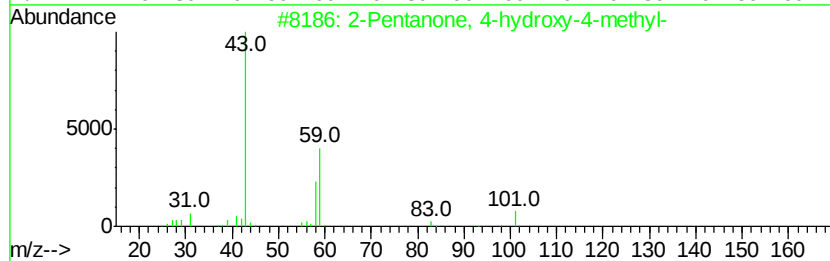
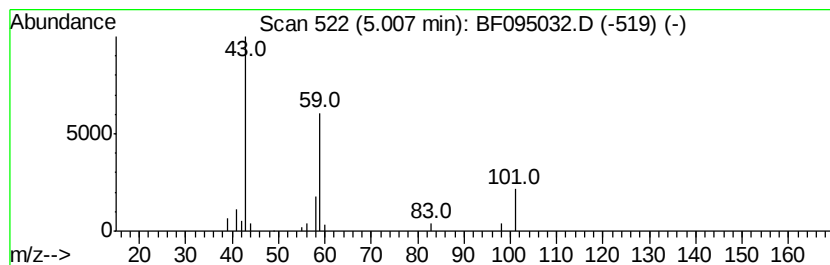
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.01	3.35 ng	82789	1,4-Dichlorobenzene-d4	7.71

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	23
3		2-Propyn-1-ol, acetate	98	C5H6O2	000627-09-8	9
4		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	9
5		2-Nonanone, 9-hydroxy-	158	C9H18O2	025368-56-3	9



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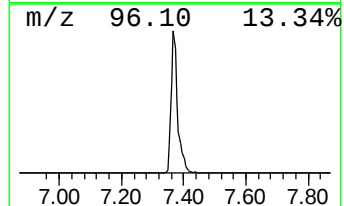
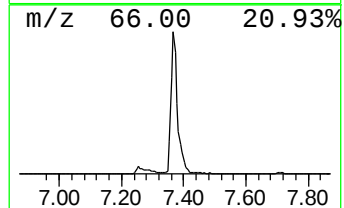
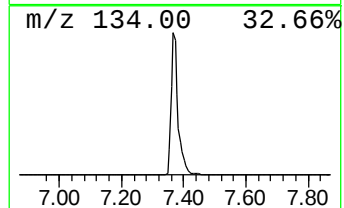
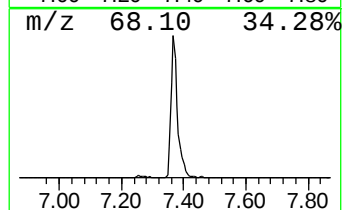
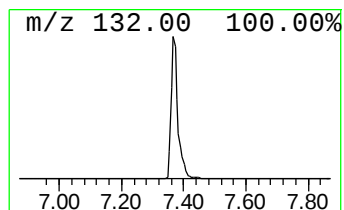
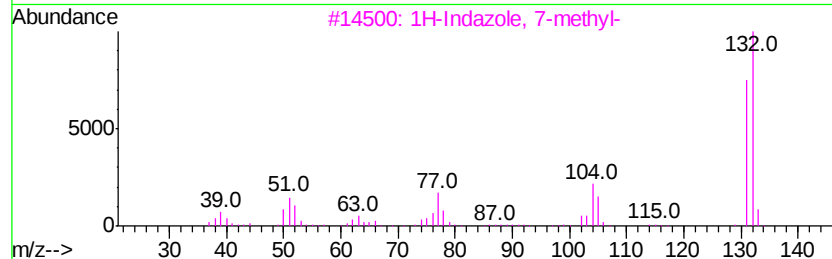
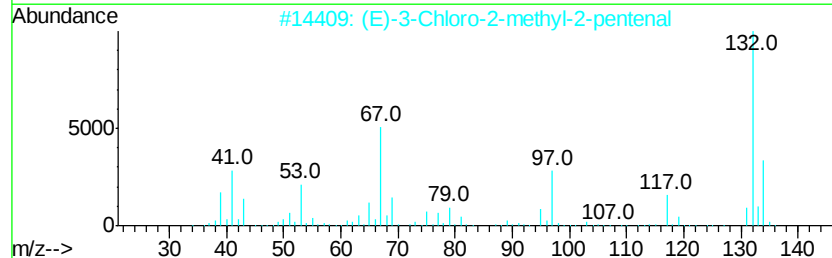
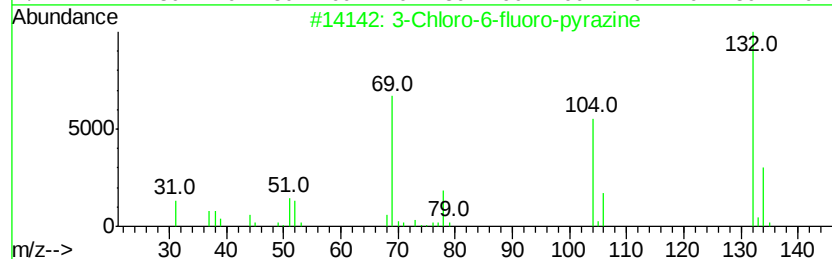
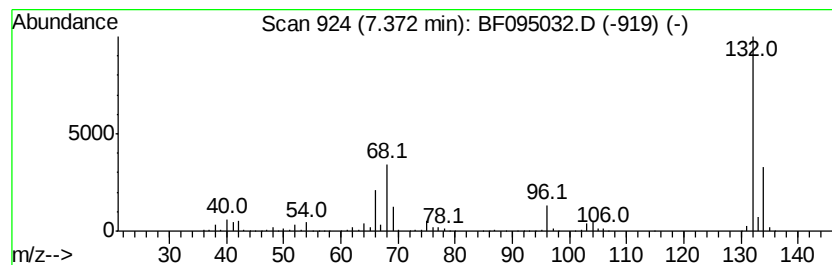
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown7.37 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.37	65.28 ng	1613840	1,4-Dichlorobenzene-d4	7.71

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	25
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3		1H-Indazole, 7-methyl-	132	C8H8N2	1000316-00-7	10
4		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	10
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9



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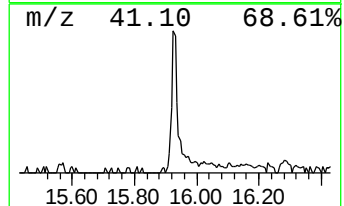
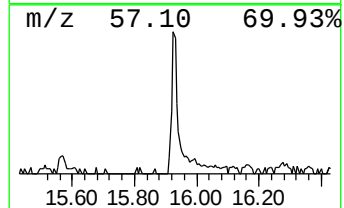
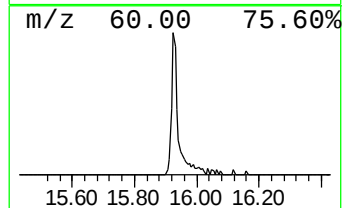
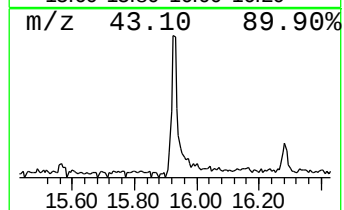
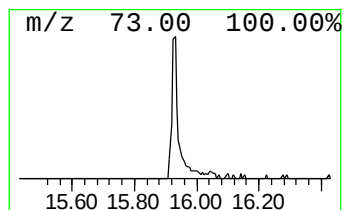
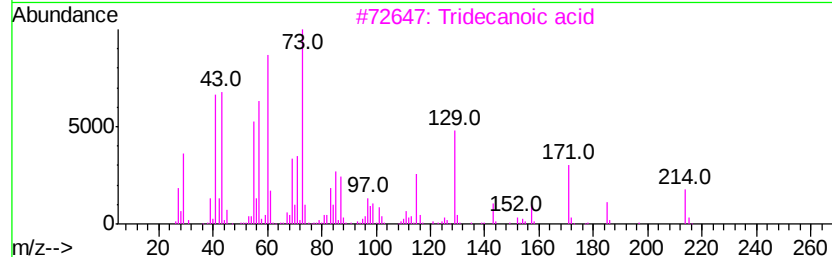
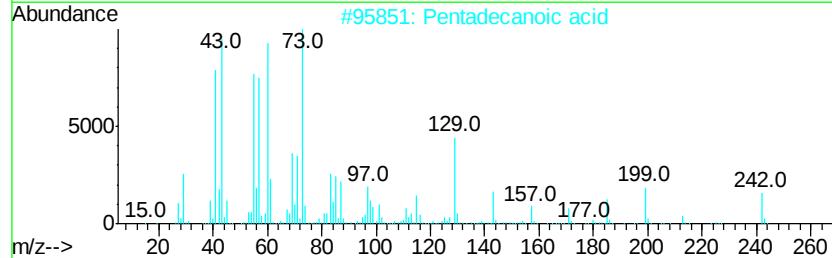
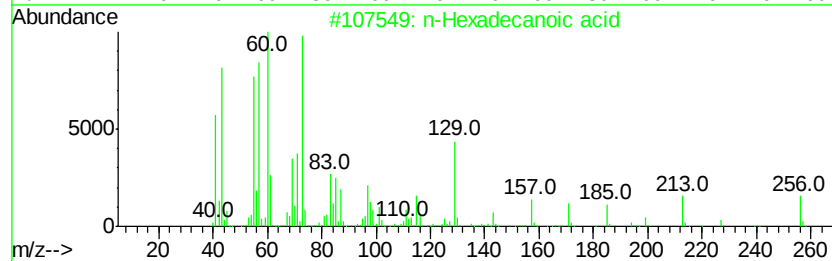
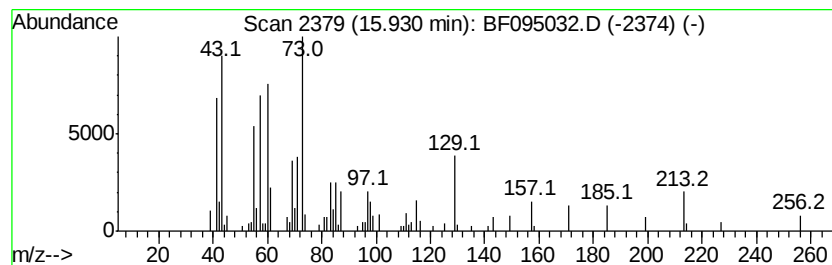
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.93	5.03 ng	195168	Phenanthrene-d10	14.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	83
3	Tridecanoic acid	214	C13H26O2	000638-53-9	76
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5	Dodecanoic acid	200	C12H24O2	000143-07-7	50



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Misc :
ALS Vial : 9 Sample Multiplier: 1

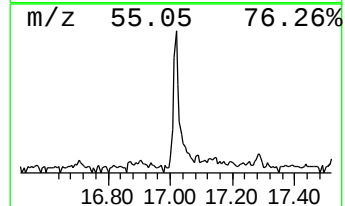
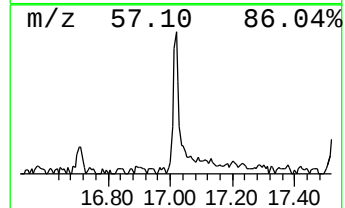
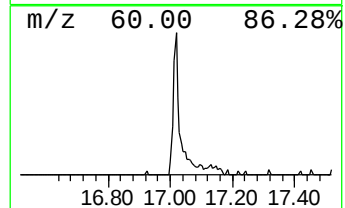
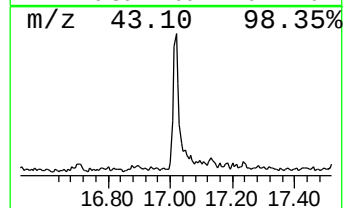
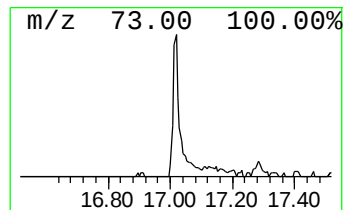
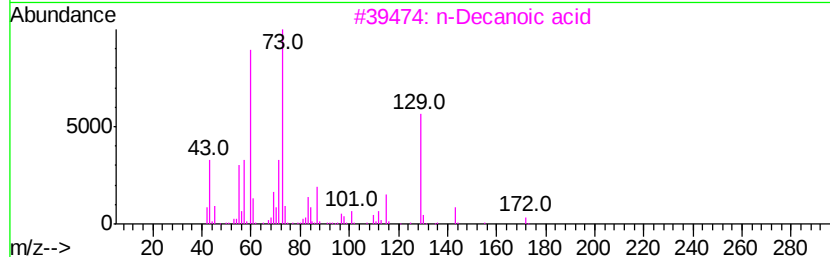
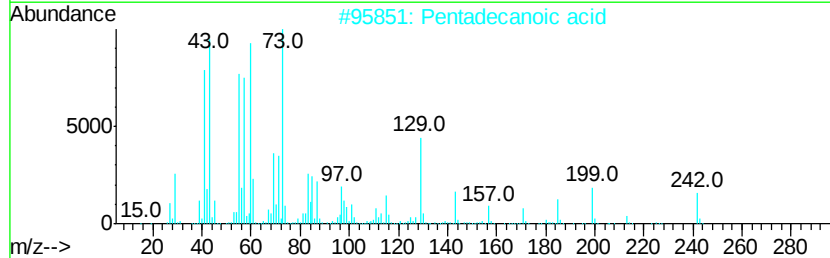
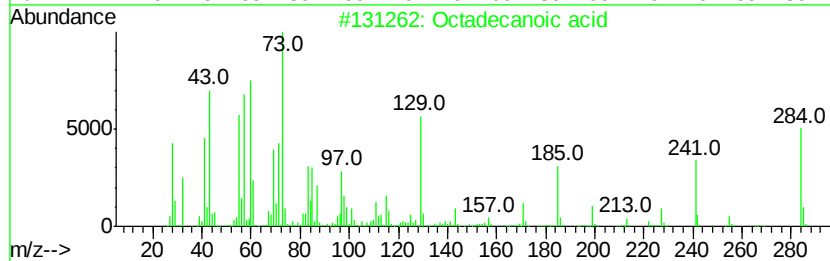
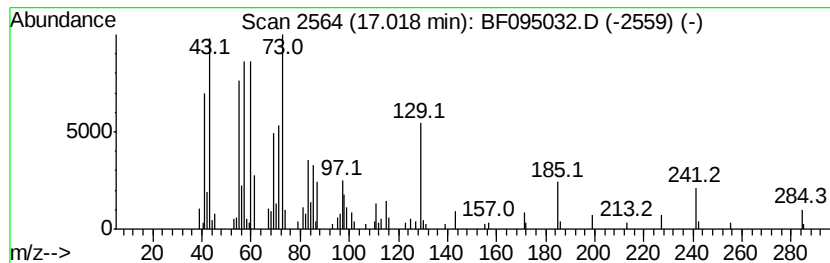
Instrument :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Octadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
17.02	6.79 ng	226906	Chrysene-d12	18.63	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3	n-Decanoic acid	172	C10H20O2	000334-48-5	78
4	Octadecanoic acid, 2-(2-hydroxyve...	372	C22H44O4	000106-11-6	72
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	68



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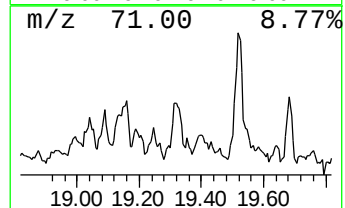
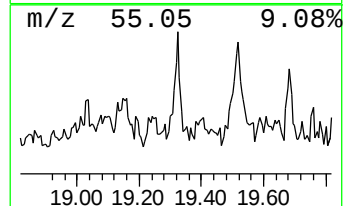
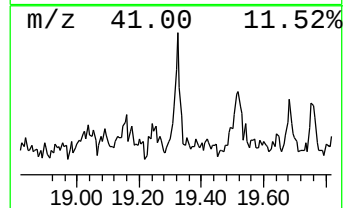
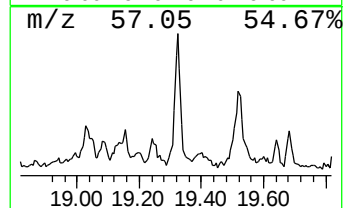
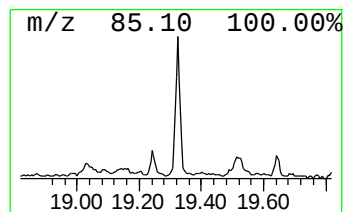
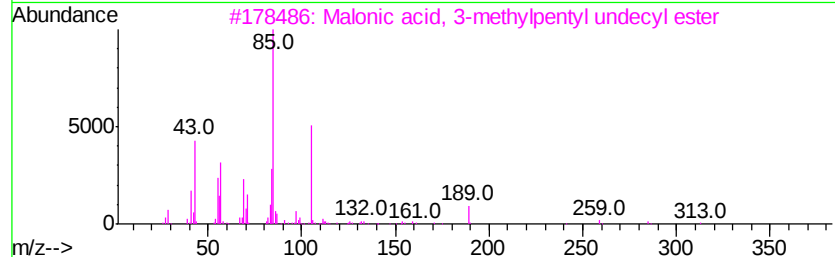
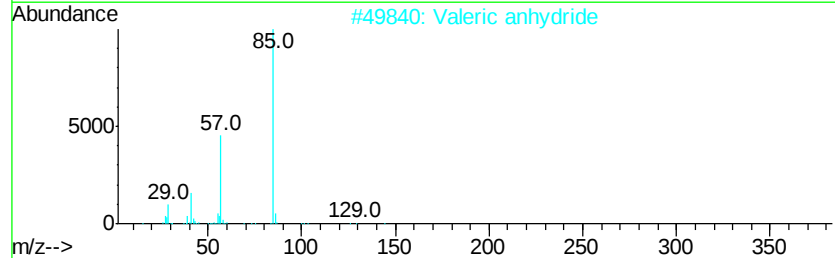
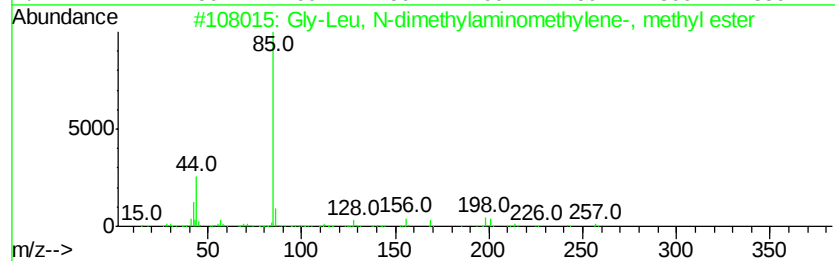
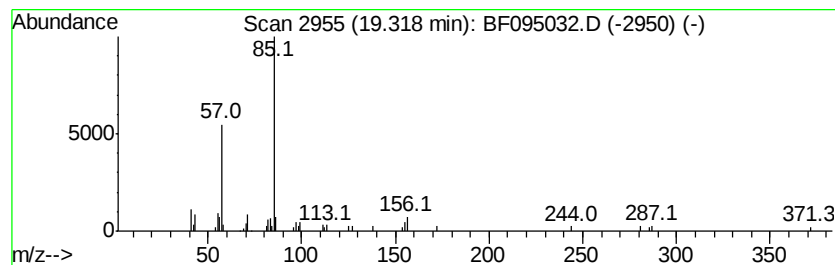
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Peak Number 6 Gly-Leu, N-dimethylaminomet... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.32	2.37 ng	79121	Chrysene-d12	18.63

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Gly-Leu, N-dimethylaminomethylen...	257	C12H23N3O3	1000375-72-0	64
2		Valeric anhydride	186	C10H18O3	002082-59-9	59
3		Malonic acid, 3-methylpentyl undecyl...	342	C20H38O4	1000348-28-5	45
4		1,2-Benzenediol, 0-pentafluoropropyl...	340	C14H13F5O4	1000329-76-2	45
5		Valeric acid, 4-cyanophenyl ester	203	C12H13NO2	1000307-98-7	45



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Sample : I3014-04
Misc :
ALS Vial : 9 Sample Multiplier: 1

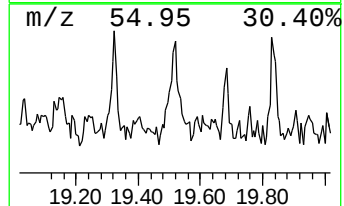
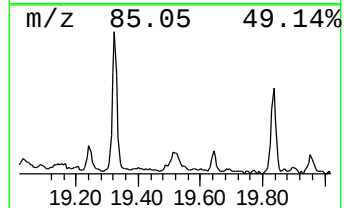
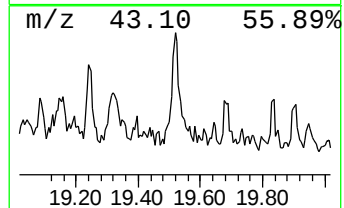
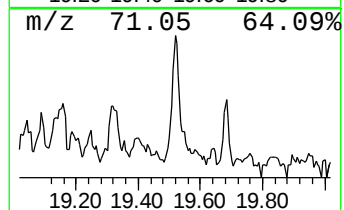
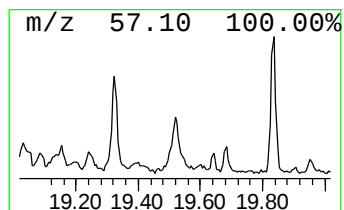
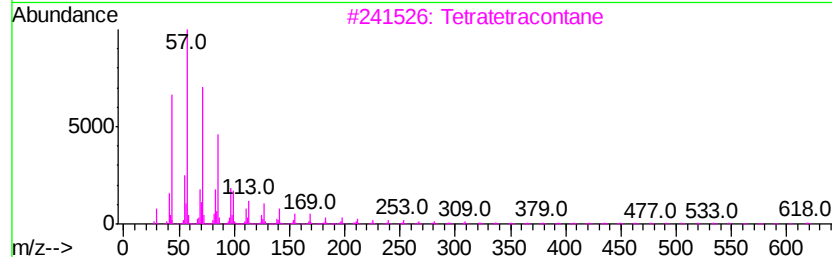
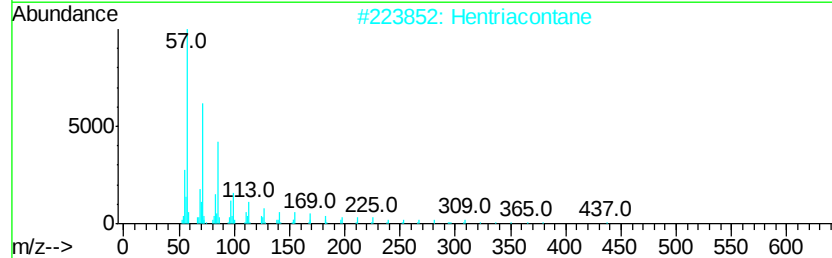
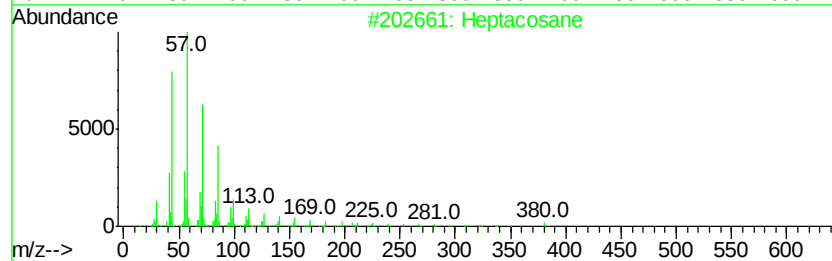
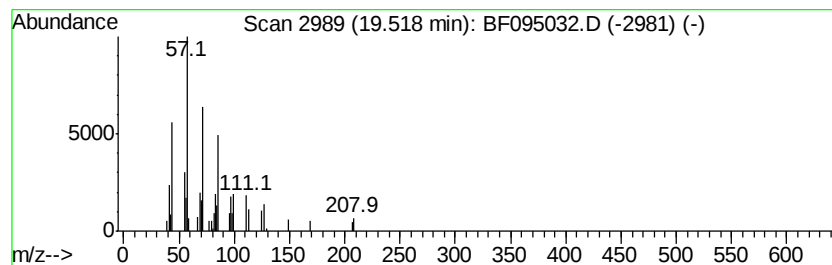
Instrument :
BNA_F
ClientSampleId :
RAV-GTMW-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Heptacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.52	2.49 ng	68401	Perylene-d12	20.29
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Heptacosane	380 C27H56	000593-49-7	80
2	Hentriacontane	437 C31H64	000630-04-6	80
3	Tetratetracontane	619 C44H90	007098-22-8	78
4	10-Methylnonadecane	282 C20H42	056862-62-5	72
5	2-methyloctacosane	408 C29H60	1000376-72-8	72



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050917\
Data File : BF095032.D
Acq On : 9 May 2017 20:39
Operator : SJ/MA
Sample : I3014-04
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RAV-GTMW-3

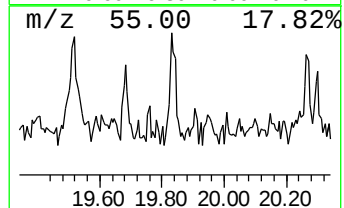
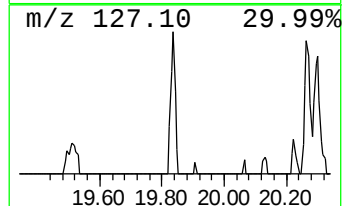
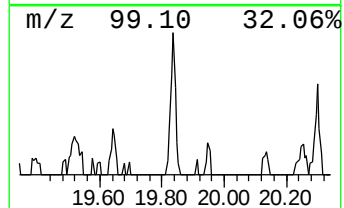
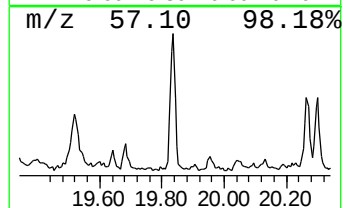
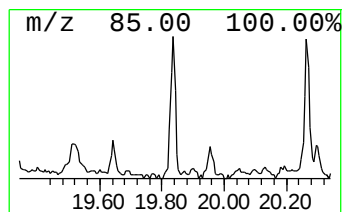
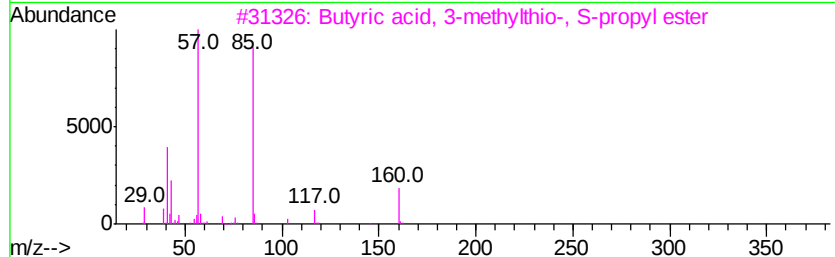
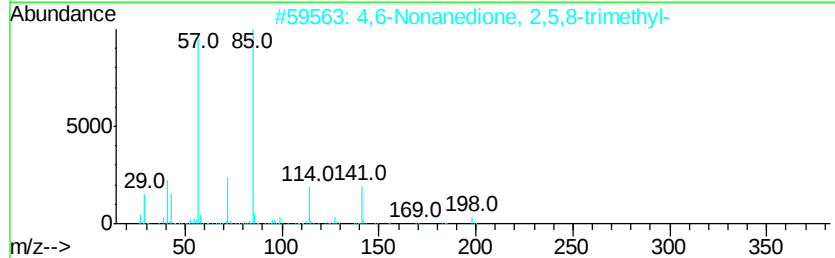
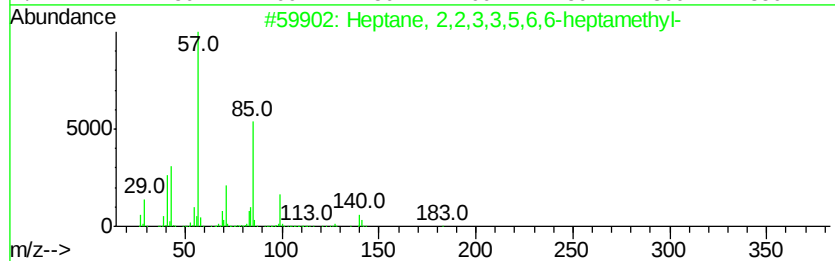
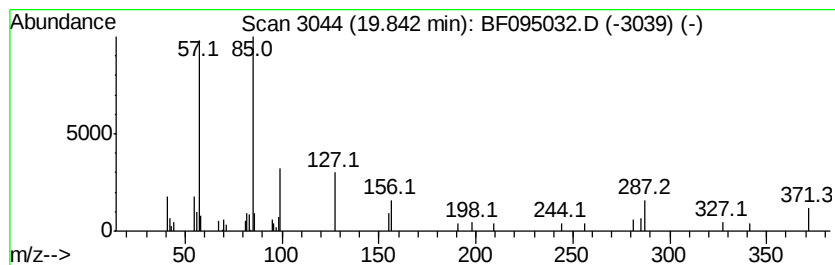
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Heptane, 2,2,3,3,5,6,6-hept... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.84	2.59 ng	71222	Perylene-d12	20.29

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptane, 2,2,3,3,5,6,6-heptamethyl-	198	C14H30	007225-67-4	53
2		4,6-Nonanedione, 2,5,8-trimethyl-	198	C12H22O2	1000162-14-3	47
3		Butyric acid, 3-methylthio-, S-p...	160	C8H16OS	002432-58-8	43
4		Decane, 1-iodo-	268	C10H21I	002050-77-3	42
5		2-Iodomethyl-5-methyltetrahydrof...	226	C6H11IO	019056-49-6	40



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050917\
Data File : BF095032.D
Acq On : 9 May 2017 20:39
Operator : SJ/MA
Sample : I3014-04
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RAV-GTMW-3

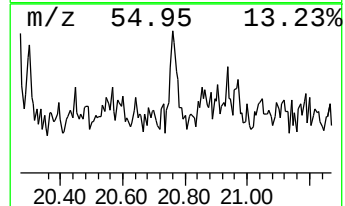
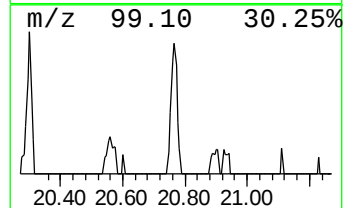
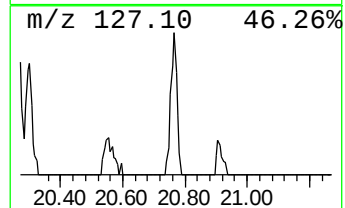
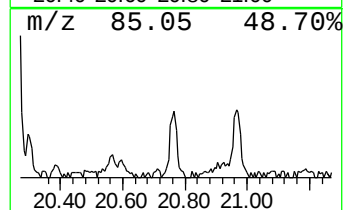
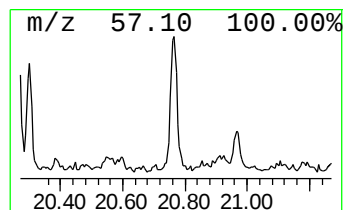
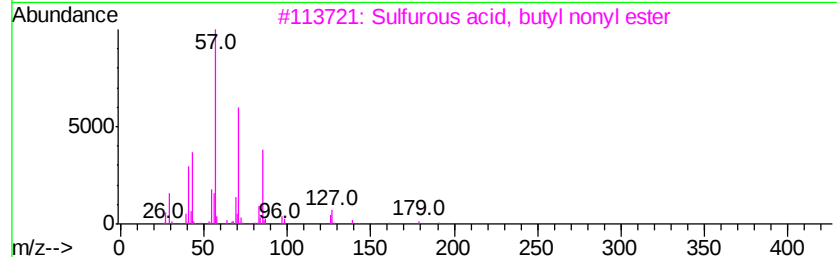
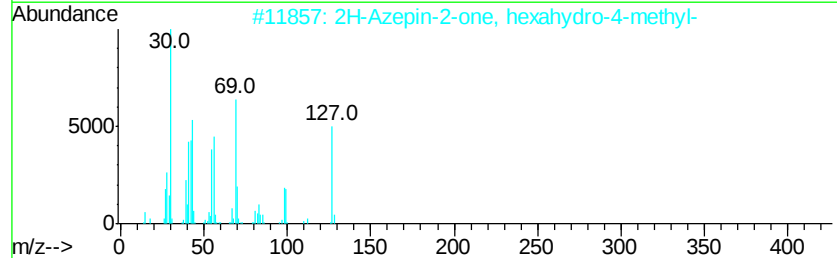
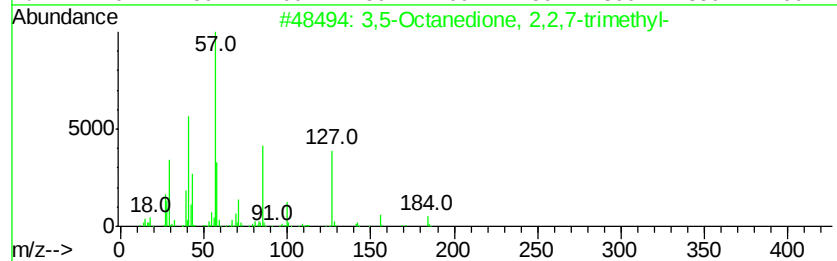
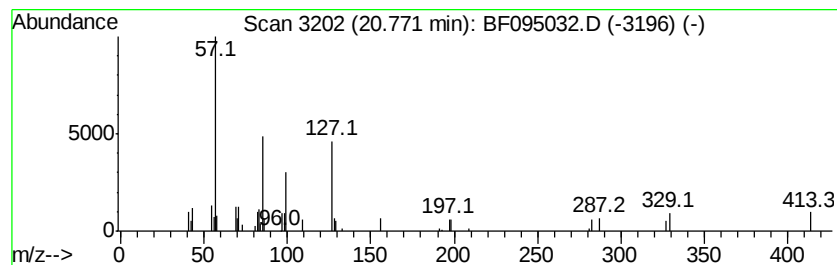
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown20.77 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.77	2.14 ng	58845	Perylene-d12	20.29

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3,5-Octanedione, 2,2,7-trimethyl-	184	C11H20O2	069725-37-7	38
2		2H-Azepin-2-one, hexahydro-4-met...	127	C7H13NO	003623-05-0	35
3		Sulfurous acid, butyl nonyl ester	264	C13H28O3S	1000309-17-6	35
4		Tridecane, 1-iodo-	310	C13H27I	035599-77-0	27
5		Eicosane	282	C20H42	000112-95-8	27



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050917\
Data File : BF095032.D
Acq On : 9 May 2017 20:39
Operator : SJ/MA
Sample : I3014-04
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RAV-GTMW-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.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...	5.01	3.4	ng	82789	1	7.71	494401	20.0
unknown7.37	7.37	65.3	ng	1613840	1	7.71	494401	20.0
n-Hexadecanoic acid	15.93	5.0	ng	195168	4	14.96	775732	20.0
Octadecanoic acid	17.02	6.8	ng	226906	5	18.63	667900	20.0
Gly-Leu, N-dimeth...	19.32	2.4	ng	79121	5	18.63	667900	20.0
Heptacosane	19.52	2.5	ng	68401	6	20.29	550314	20.0
Heptane, 2,2,3,3,...	19.84	2.6	ng	71222	6	20.29	550314	20.0
unknown20.77	20.77	2.1	ng	58845	6	20.29	550314	20.0