

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF042919\
 Data File : BF114021.D
 Acq On : 29 Apr 2019 13:39
 Operator : JU/SJ
 Sample : K2576-01
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MW-16

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-BF042219.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	2.187	13	17	29	rVB	198056	292770	7.12%	0.888%
2	5.510	578	582	600	rBV	1409617	1447317	35.19%	4.388%
3	6.516	749	753	764	rVB	1040515	940841	22.88%	2.852%
4	6.663	773	778	781	rBV	2979603	2683232	65.24%	8.135%
5	6.892	813	817	821	rBV	923622	749396	18.22%	2.272%
6	7.051	840	844	847	rBV	2800947	2370912	57.65%	7.188%
7	7.451	907	912	915	rBV	2013902	1947150	47.34%	5.903%
8	8.175	1031	1035	1041	rBV	992189	939305	22.84%	2.848%
9	8.833	1144	1147	1151	rBV4	31021	52753	1.28%	0.160%
10	9.010	1173	1177	1182	rVB7	32783	59827	1.45%	0.181%
11	9.245	1212	1217	1220	rBV	4284055	3937397	95.74%	11.937%
12	9.827	1312	1316	1320	rBV6	37791	61626	1.50%	0.187%
13	9.922	1329	1332	1336	rBV	1291519	1175941	28.59%	3.565%
14	10.710	1462	1466	1481	rBV	2435232	2631824	63.99%	7.979%
15	11.410	1581	1585	1588	rBV	1212194	1109469	26.98%	3.364%
16	11.945	1670	1676	1687	rBV	1672382	1879602	45.70%	5.698%
17	12.639	1789	1794	1802	rBV3	109796	237722	5.78%	0.721%
18	12.739	1803	1811	1828	rVV	2950462	4112732	100.00%	12.469%
19	12.992	1850	1854	1858	rBV	3822241	3935477	95.69%	11.931%
20	14.068	2033	2037	2046	rVB	965655	892978	21.71%	2.707%
21	14.568	2117	2122	2127	rVB2	43653	55123	1.34%	0.167%
22	14.892	2174	2177	2181	rVB	78299	73374	1.78%	0.222%
23	15.239	2232	2236	2244	rVB	92545	115825	2.82%	0.351%
24	15.586	2290	2295	2299	rBV	706096	924359	22.48%	2.802%
25	15.627	2299	2302	2308	rVB	106819	143828	3.50%	0.436%
26	16.074	2373	2378	2383	rBV	80756	122301	2.97%	0.371%
27	16.592	2461	2466	2477	rVB2	48681	91836	2.23%	0.278%

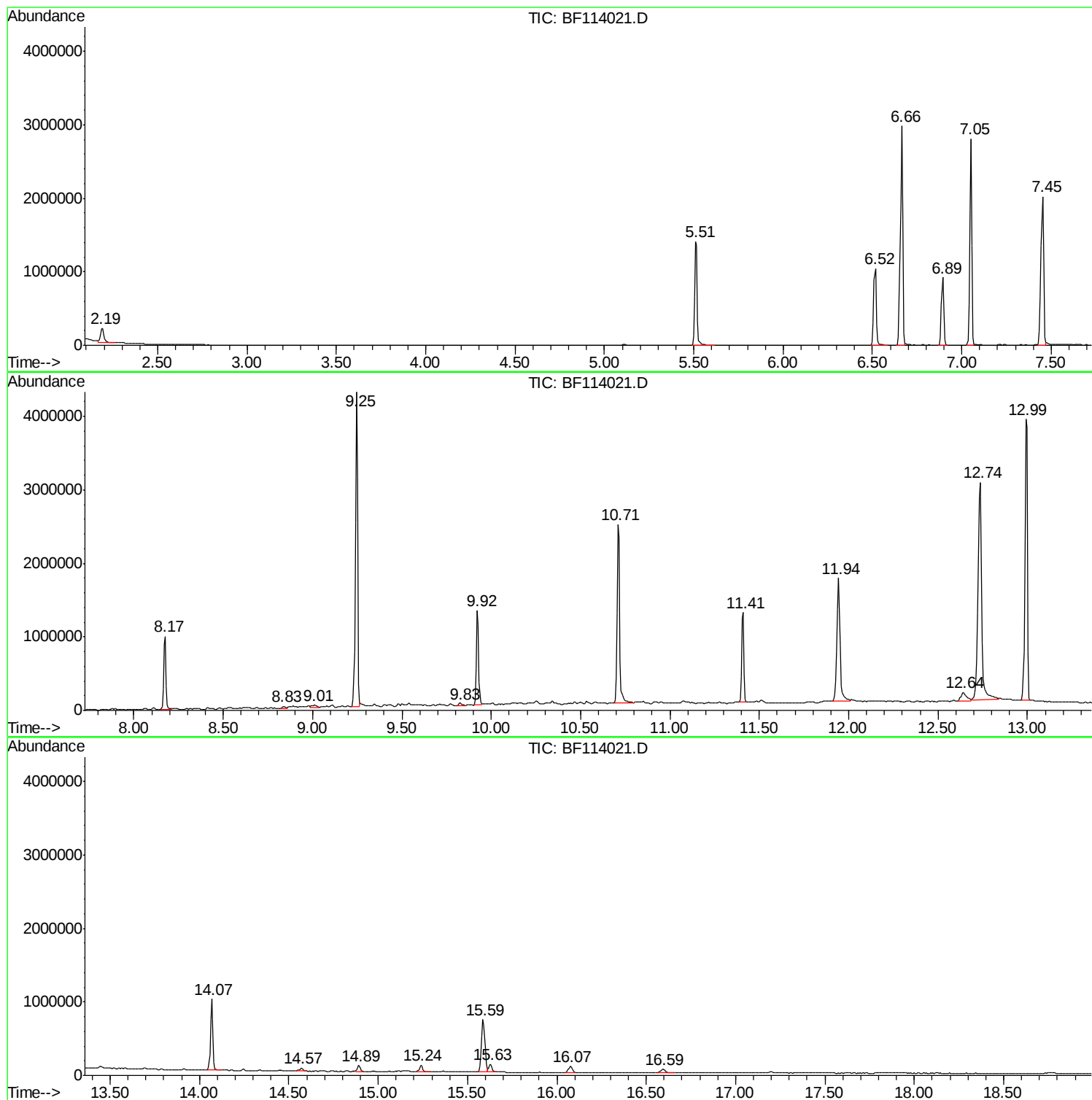
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF042219.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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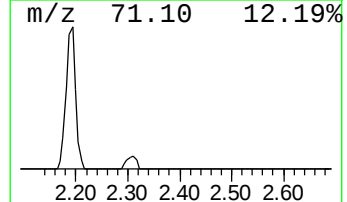
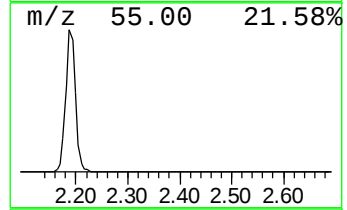
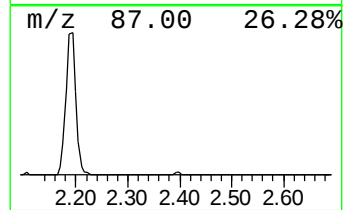
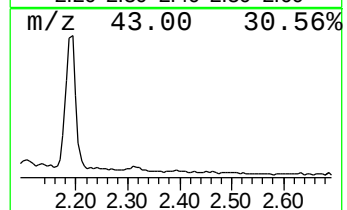
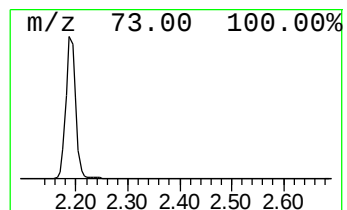
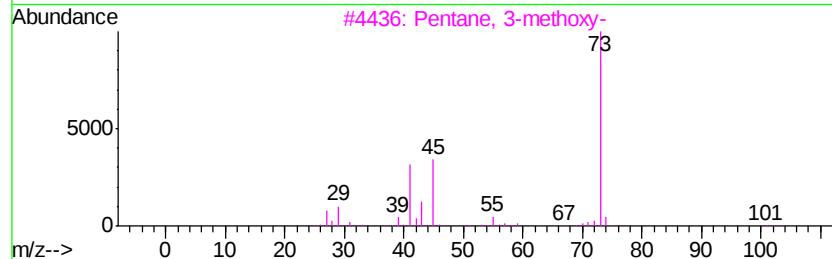
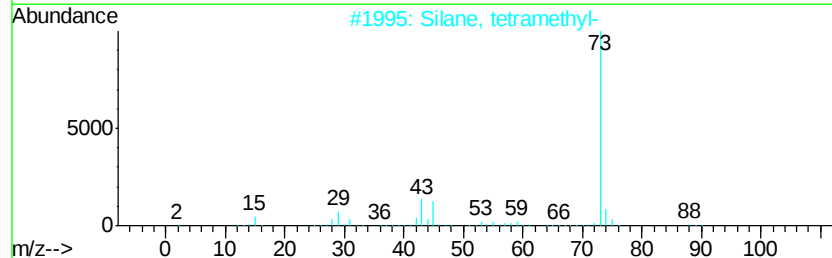
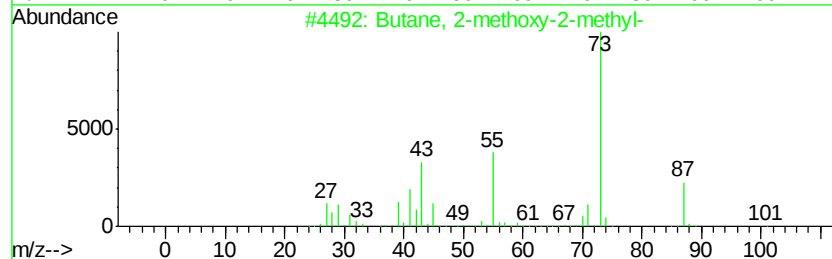
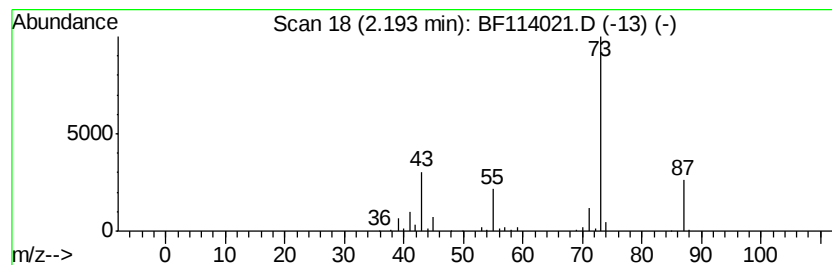
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.19	7.81 ng	292770	1,4-Dichlorobenzene-d4	6.89

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	64
2		Silane, tetramethyl-	88	C4H12Si	000075-76-3	35
3		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
4		Borane, dimethoxy-	74	C2H7BO2	004542-61-4	9
5		N-Ethylformamide	73	C3H7NO	000627-45-2	9



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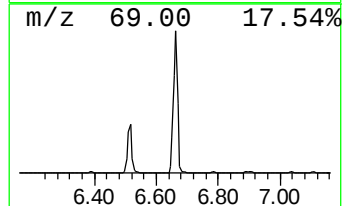
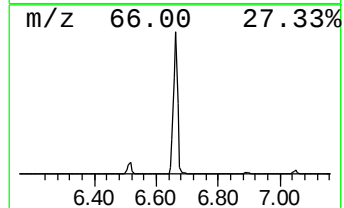
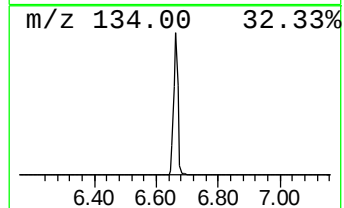
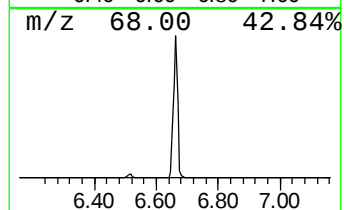
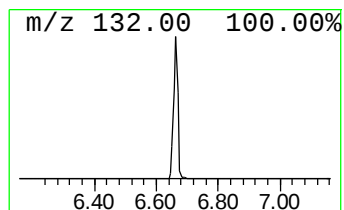
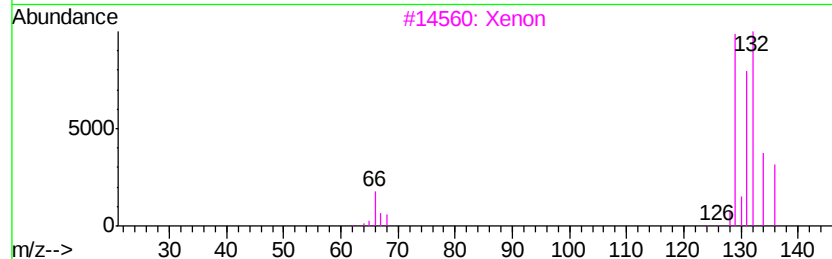
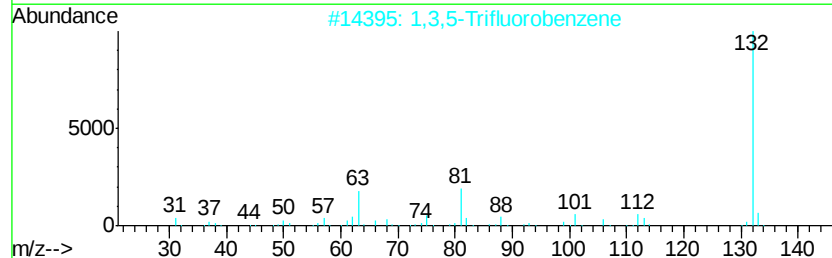
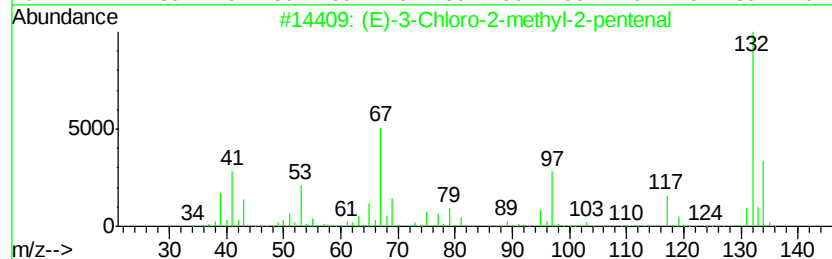
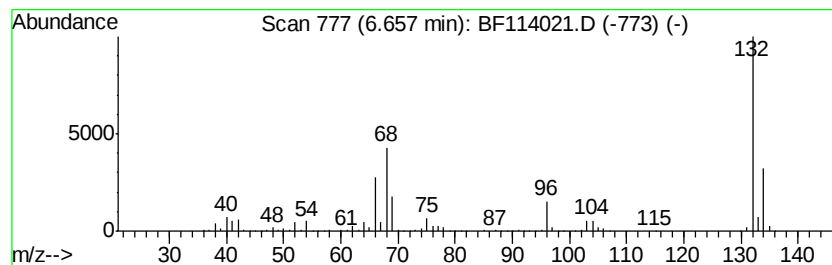
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Peak Number 2 unknown6.66 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.66	71.61 ng	2683230	1,4-Dichlorobenzene-d4	6.89

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
2		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
3		Xenon	132	Xe	007440-63-3	9
4		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9



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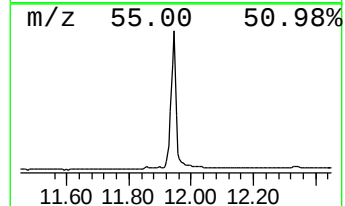
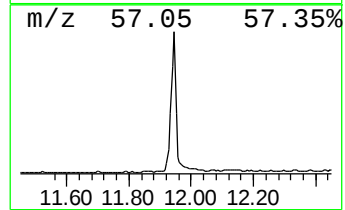
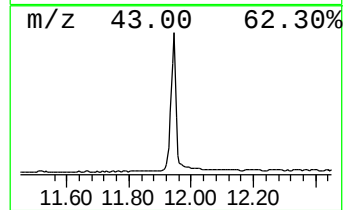
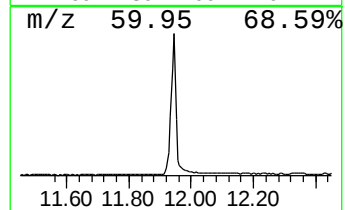
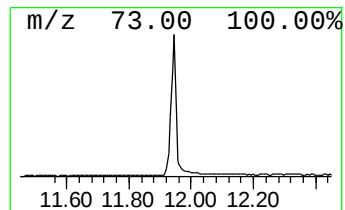
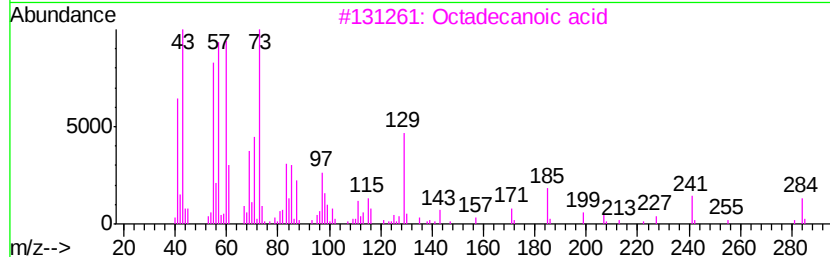
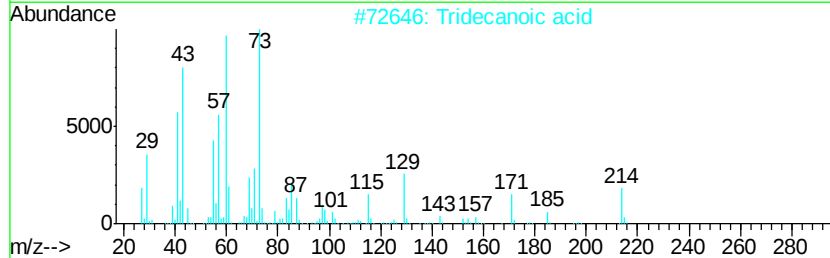
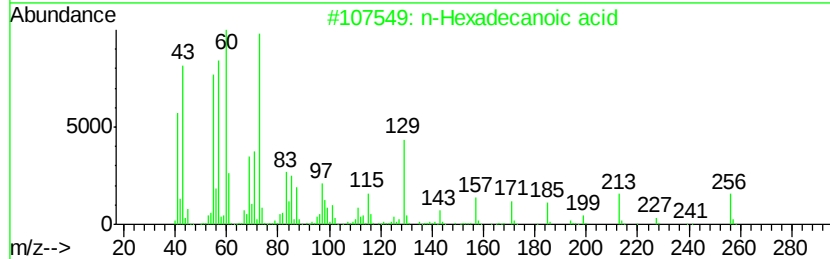
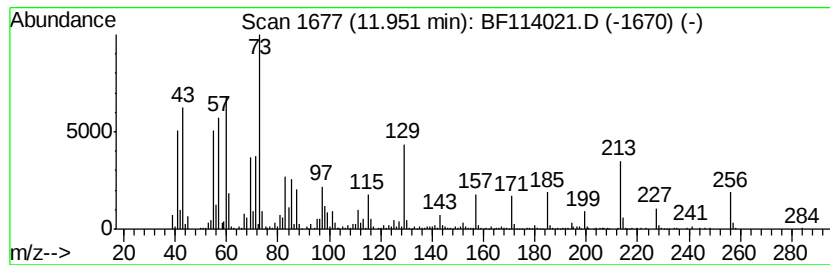
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.95	33.88 ng	1879600	Phenanthrene-d10	11.41

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	90
3		Octadecanoic acid	284	C18H36O2	000057-11-4	87
4		Pentadecanoic acid	242	C15H30O2	001002-84-2	81
5		n-Decanoic acid	172	C10H20O2	000334-48-5	70



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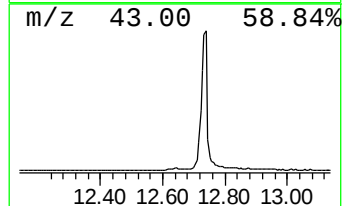
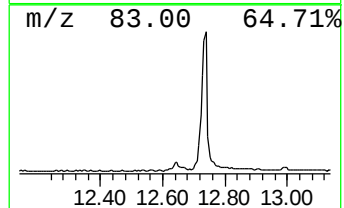
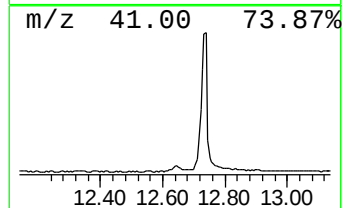
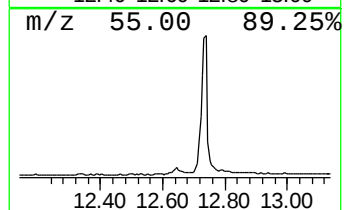
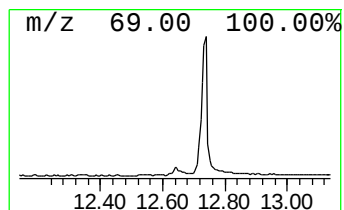
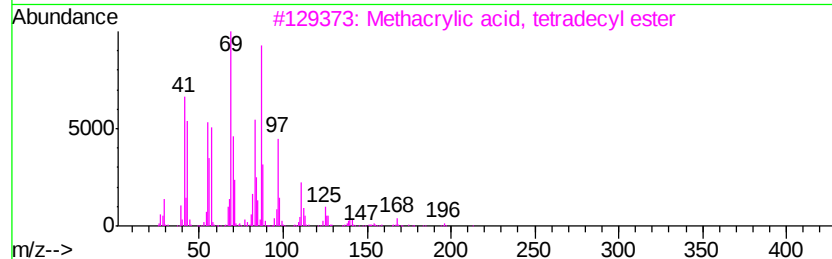
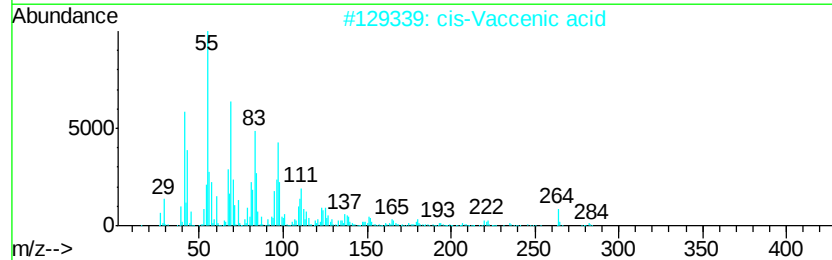
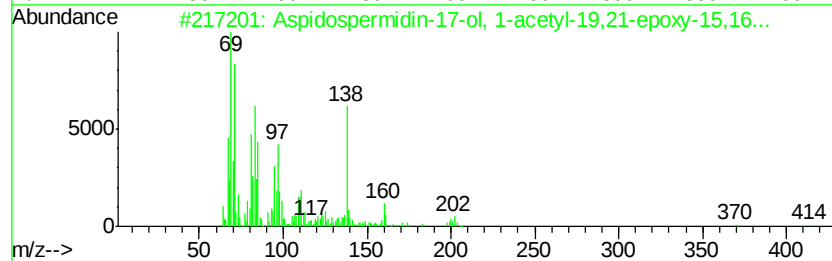
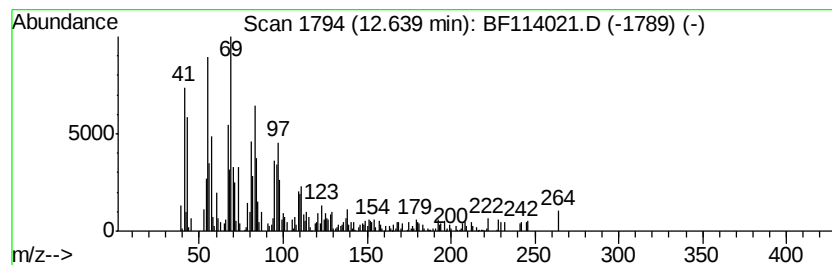
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Peak Number 5 Aspidospermidin-17-ol, 1-ac... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.64	4.29 ng	237722	Phenanthrene-d10	11.41

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Aspidospermidin-17-ol, 1-acetyl-...	414	C23H30N2O5	002122-26-1	87
2		cis-Vaccenic acid	282	C18H34O2	000506-17-2	53
3		Methacrylic acid, tetradecyl ester	282	C18H34O2	1000340-29-0	53
4		Oleic Acid	282	C18H34O2	000112-80-1	53
5		5-Tetradecene, (E)-	196	C14H28	041446-66-6	53



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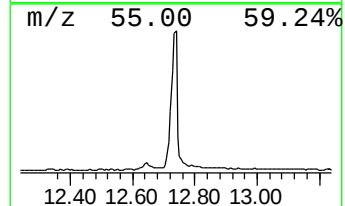
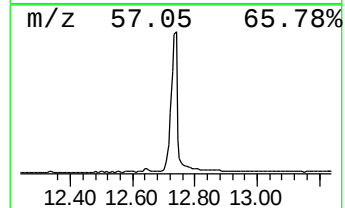
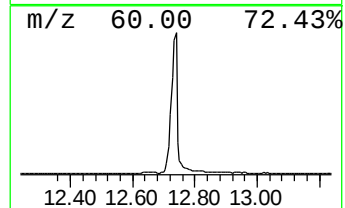
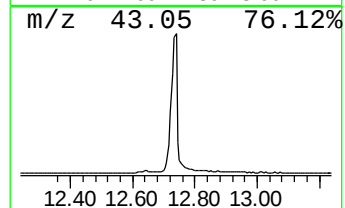
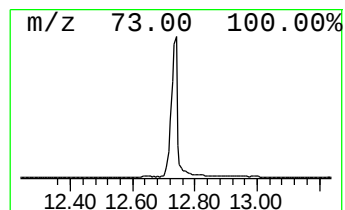
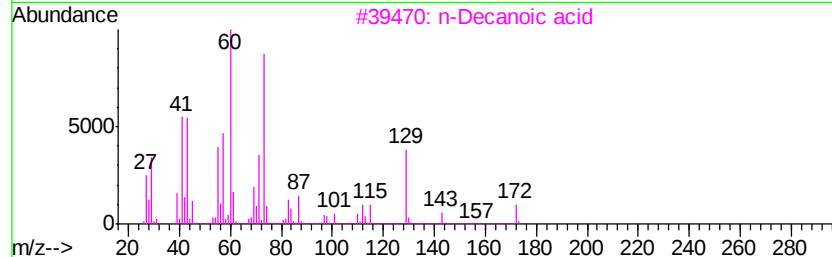
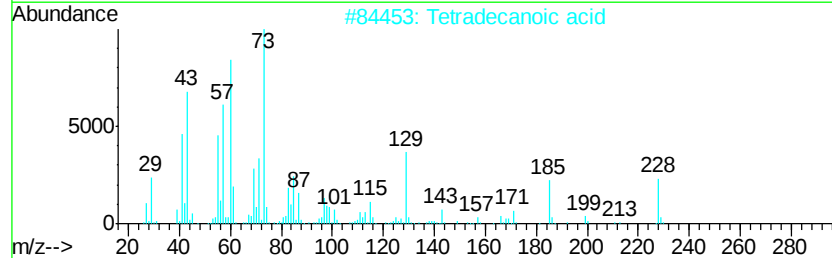
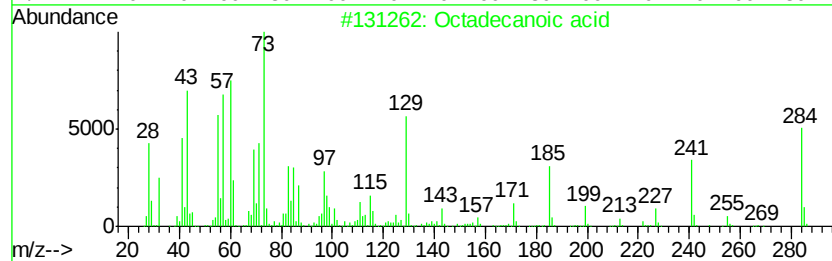
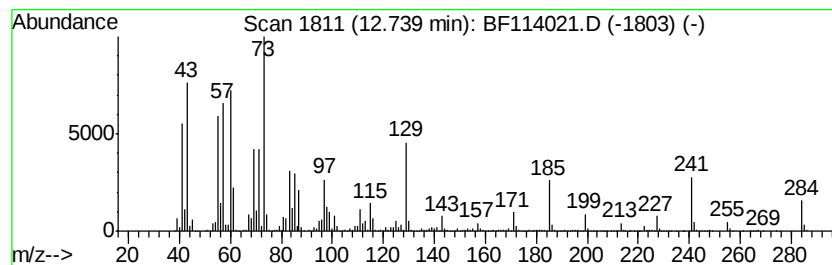
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 Peak Number 6 Octadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD		R.T.	
12.74	92.11 ng	4112730	Chrysene-d12		14.07	
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octadecanoic acid	284	C18H36O2	000057-11-4	99
2		Tetradecanoic acid	228	C14H28O2	000544-63-8	74
3		n-Decanoic acid	172	C10H20O2	000334-48-5	58
4		Pentadecanoic acid	242	C15H30O2	001002-84-2	53
5		Hexadecane	226	C16H34	000544-76-3	25



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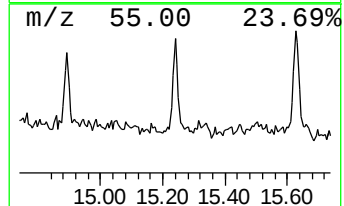
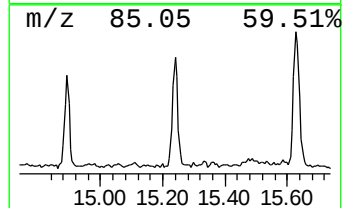
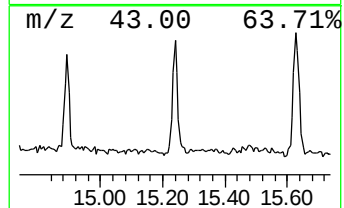
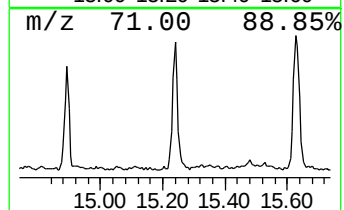
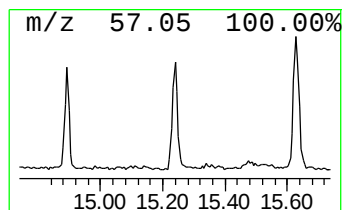
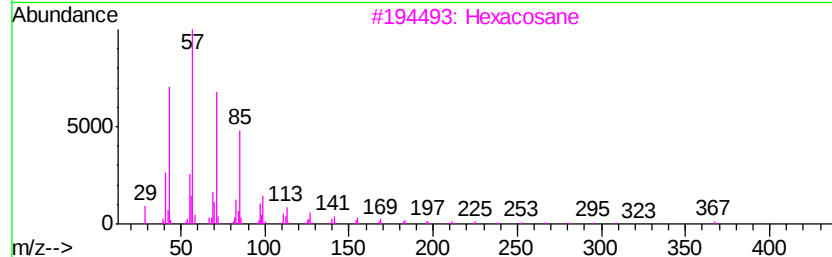
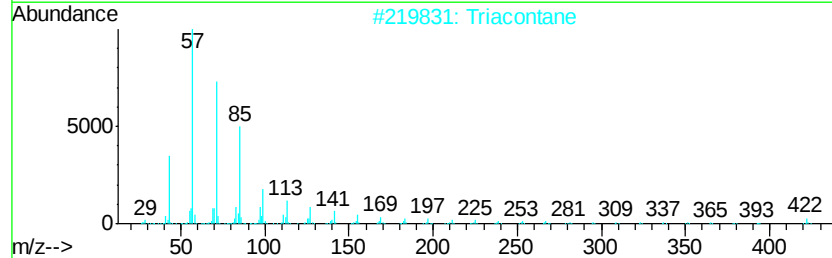
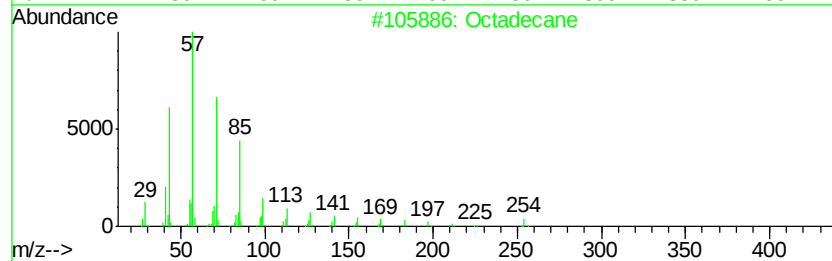
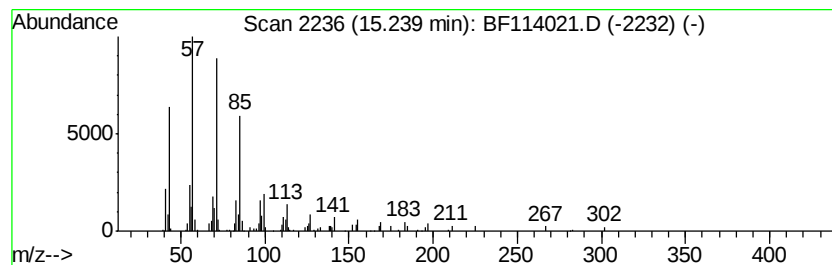
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Octadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.24	2.51 ng	115825	Perylene-d12	15.59

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane		254	C18H38	000593-45-3	91
2	triacontane		422	C30H62	000638-68-6	91
3	Hexacosane		366	C26H54	000630-01-3	91
4	Tetracosane		338	C24H50	000646-31-1	91
5	2-methyloctacosane		408	C29H60	1000376-72-8	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF042919\
Data File : BF114021.D
Acq On : 29 Apr 2019 13:39
Operator : JU/SJ
Sample : K2576-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-16

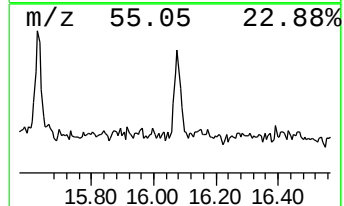
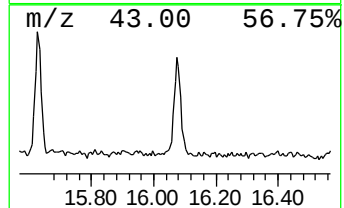
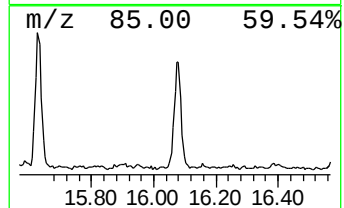
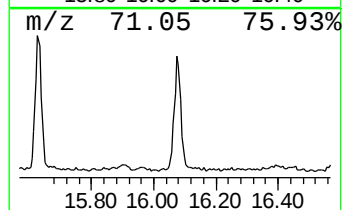
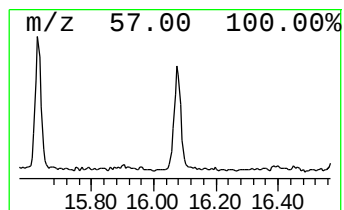
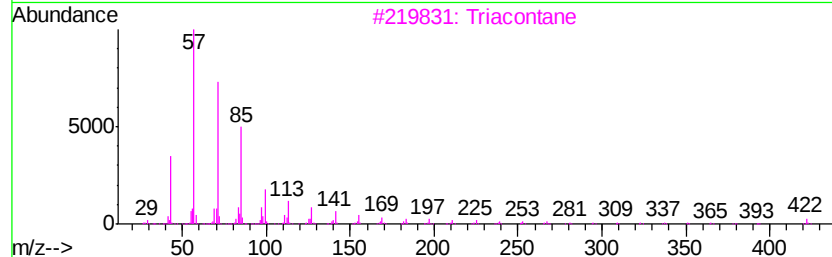
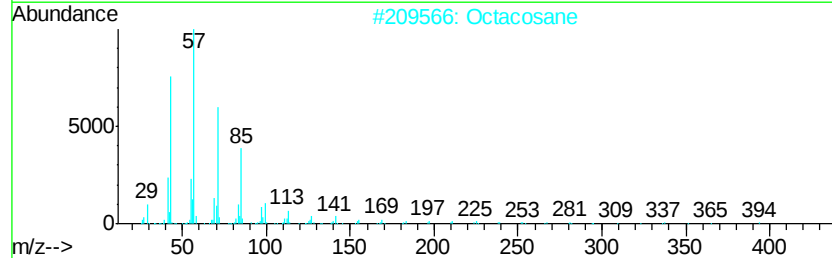
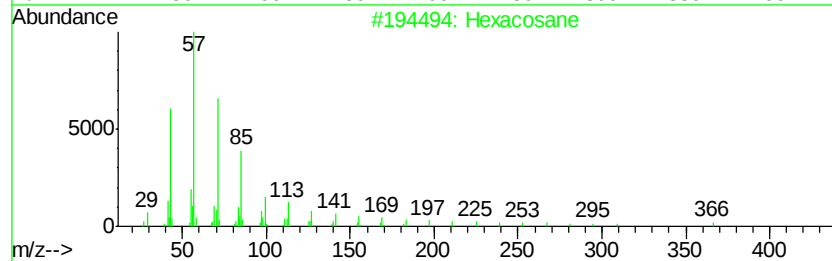
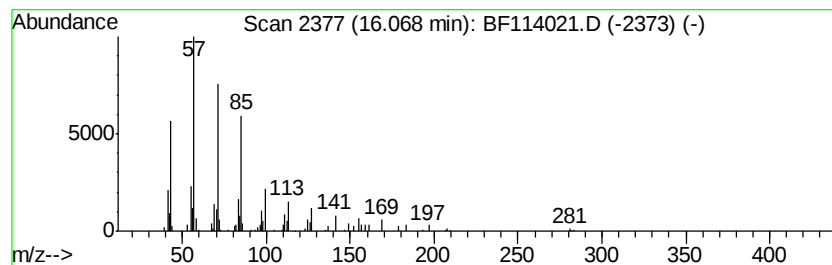
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF042219.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Hexacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.07	2.65 ng	122301	Perylene-d12	15.59

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexacosane	366	C26H54	000630-01-3	91
2		Octacosane	394	C28H58	000630-02-4	91
3		Triacotane	422	C30H62	000638-68-6	91
4		Pentacosane	352	C25H52	000629-99-2	91
5		2-methyloctacosane	408	C29H60	1000376-72-8	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF042919\
Data File : BF114021.D
Acq On : 29 Apr 2019 13:39
Operator : JU/SJ
Sample : K2576-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-16

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF042219.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...	2.19	7.8	ng	292770	1	6.89	749396	20.0
unknown6.66	6.66	71.6	ng	2683230	1	6.89	749396	20.0
n-Hexadecanoic acid	11.95	33.9	ng	1879600	4	11.41	1109470	20.0
Aspidospermidin-1...	12.64	4.3	ng	237722	4	11.41	1109470	20.0
Octadecanoic acid	12.74	92.1	ng	4112730	5	14.07	892978	20.0
Octadecane	15.24	2.5	ng	115825	6	15.59	924359	20.0
Hexacosane	16.07	2.6	ng	122301	6	15.59	924359	20.0