

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF092418\
 Data File : BF109264.D
 Acq On : 24 Sep 2018 13:49
 Operator : JU/SJ
 Sample : J5023-09
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 NB-PIT-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:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092218.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	4.252	364	368	377	rVB	28693	37763	1.35%	0.157%
2	4.899	474	478	486	rVB	137841	169676	6.05%	0.705%
3	5.322	544	550	553	rBV	2178931	2274289	81.15%	9.444%
4	6.346	719	724	735	rVB	2289888	2498143	89.13%	10.373%
5	6.475	742	746	750	rBV	2500892	2418746	86.30%	10.044%
6	6.704	782	785	789	rBV	748370	641943	22.90%	2.666%
7	6.863	808	812	815	rBV	2307543	1882451	67.17%	7.817%
8	7.269	876	881	884	rBV	1665286	1523789	54.37%	6.327%
9	7.987	999	1003	1006	rBV	1055976	816598	29.14%	3.391%
10	9.063	1182	1186	1189	rBV	3278566	2802718	100.00%	11.638%
11	9.457	1249	1253	1256	rBV	901418	670347	23.92%	2.784%
12	9.734	1297	1300	1304	rVB	1014130	912051	32.54%	3.787%
13	10.522	1429	1434	1437	rBV	1877596	1674003	59.73%	6.951%
14	11.210	1548	1551	1555	rBV	1043378	901289	32.16%	3.743%
15	11.751	1640	1643	1651	rBV2	91180	96052	3.43%	0.399%
16	12.798	1816	1821	1824	rBV	2483043	2369001	84.53%	9.837%
17	13.216	1878	1892	1893	rBV6	46740	127634	4.55%	0.530%
18	13.704	1971	1975	1984	rVB2	105230	144300	5.15%	0.599%
19	13.833	1993	1997	2001	rBV	820432	769162	27.44%	3.194%
20	14.021	2026	2029	2032	rBV	38375	35936	1.28%	0.149%
21	14.327	2077	2081	2085	rBV	46001	53146	1.90%	0.221%
22	14.621	2127	2131	2135	rBV	49420	49706	1.77%	0.206%
23	14.686	2139	2142	2146	rVB	53915	50122	1.79%	0.208%
24	14.933	2181	2184	2188	rBV	63021	63667	2.27%	0.264%
25	15.239	2230	2236	2240	rBV	708388	800712	28.57%	3.325%
26	15.286	2240	2244	2248	rVB	63350	73042	2.61%	0.303%
27	15.686	2308	2312	2318	rVB	72263	98905	3.53%	0.411%
28	16.151	2386	2391	2396	rBV2	45721	77766	2.77%	0.323%
29	16.692	2477	2483	2490	rBV2	25091	49311	1.76%	0.205%

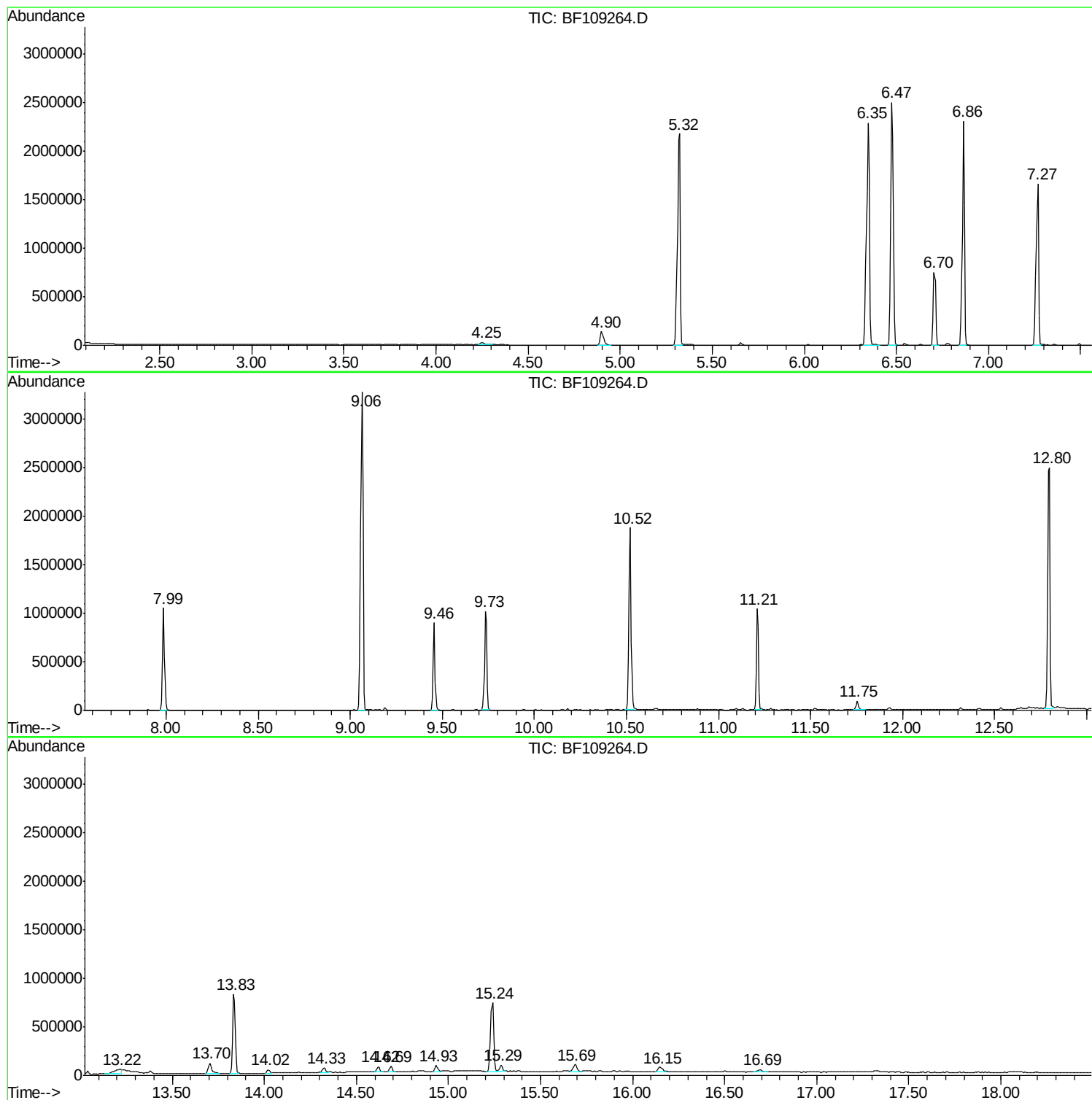
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF092218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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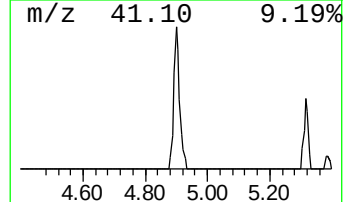
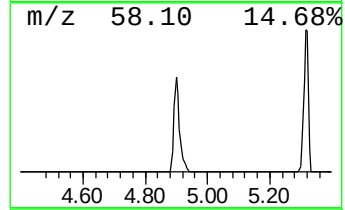
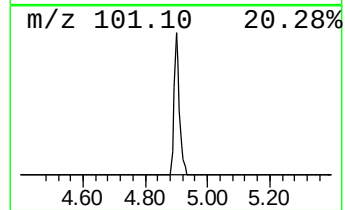
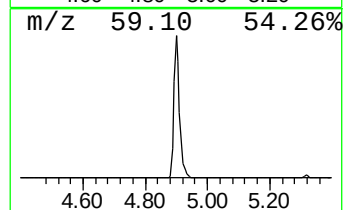
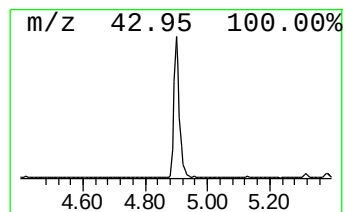
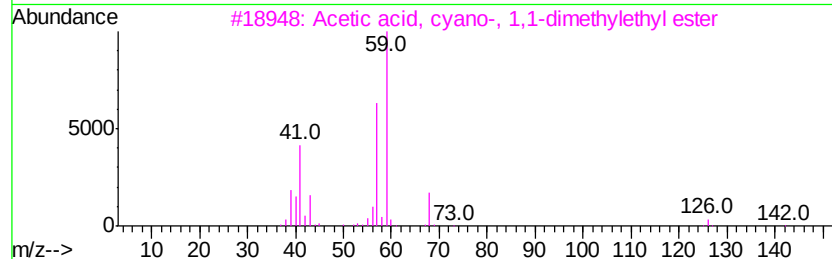
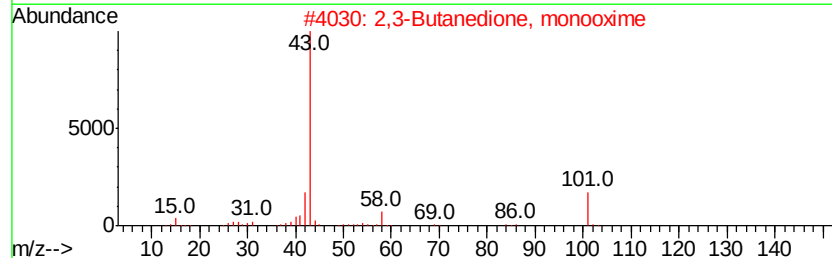
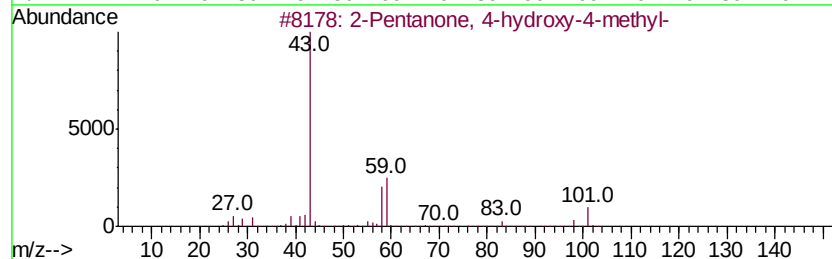
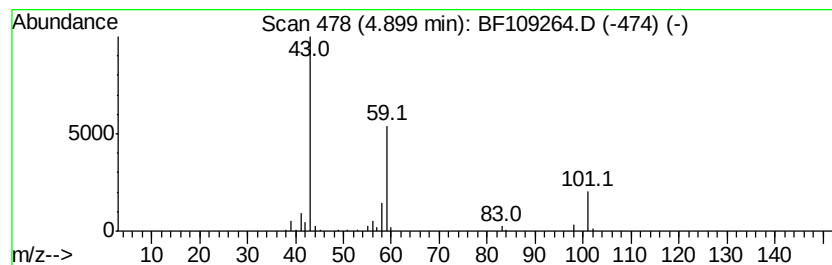
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.90	5.29 ng	169676	1,4-Dichlorobenzene-d4	6.70

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	35
3			Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	25
4			Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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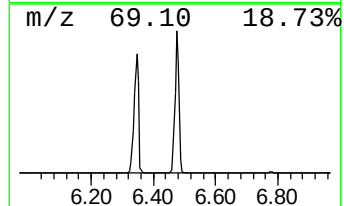
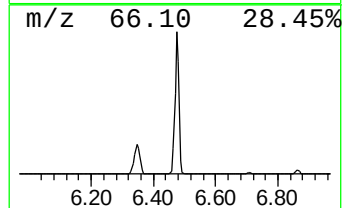
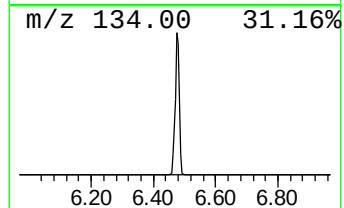
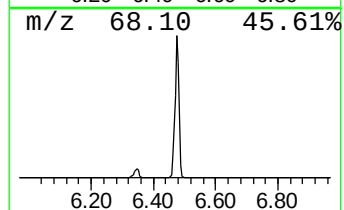
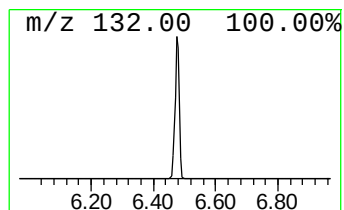
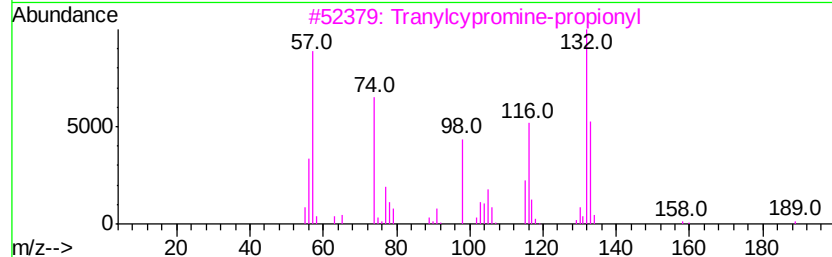
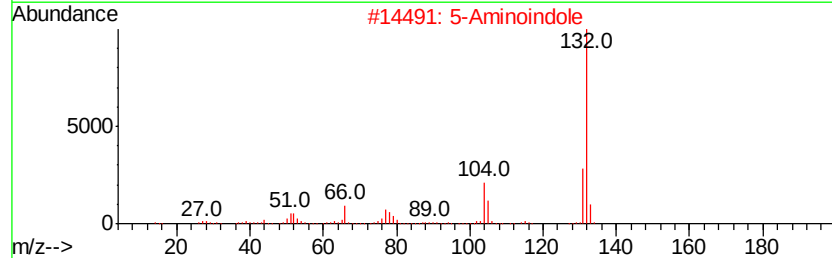
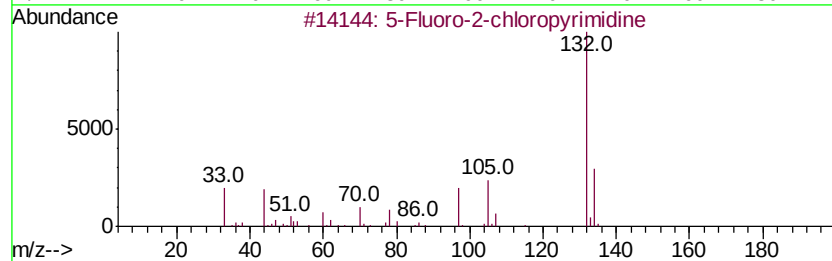
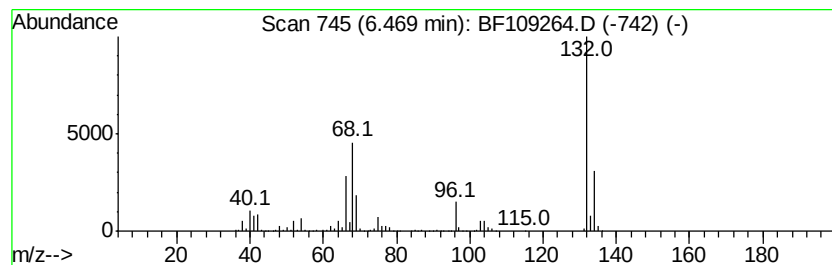
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Peak Number 2 unknown6.47 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.47	75.36 ng	2418750	1,4-Dichlorobenzene-d4	6.70

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
2			5-Aminoindole	132	C8H8N2	005192-03-0	12
3			Tranvlcyproline-propionyl	189	C12H15NO	1000123-86-3	10
4			Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9
5			2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9



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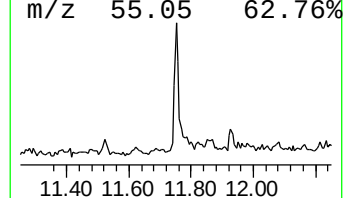
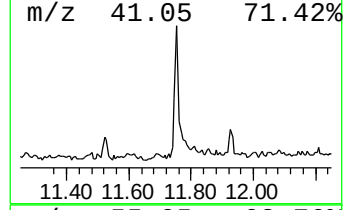
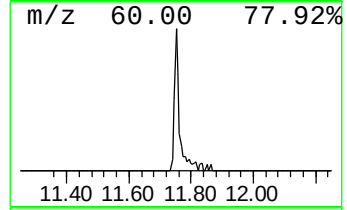
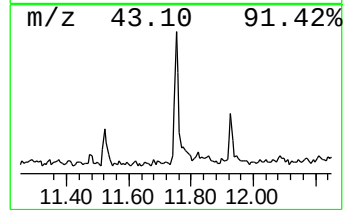
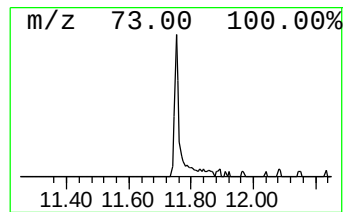
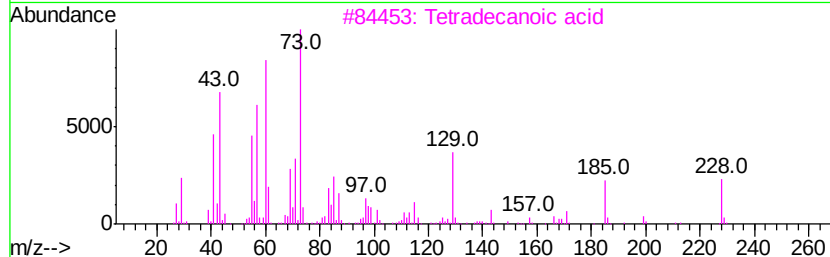
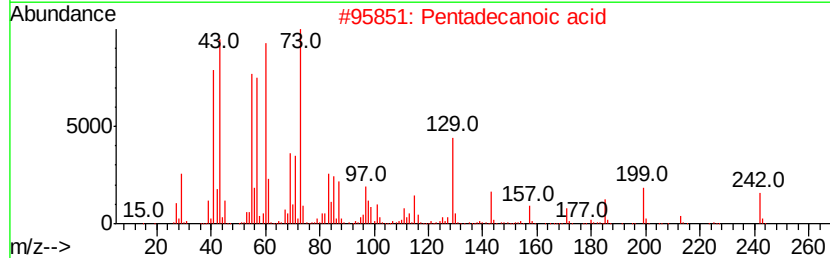
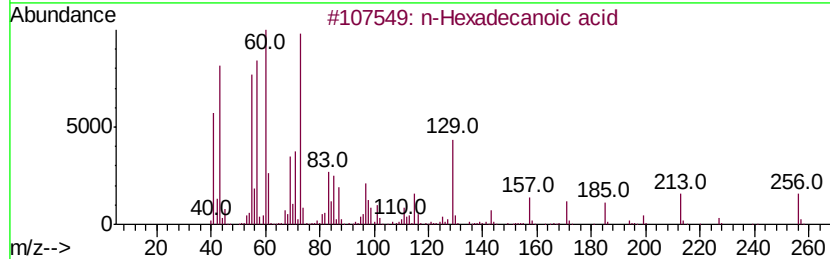
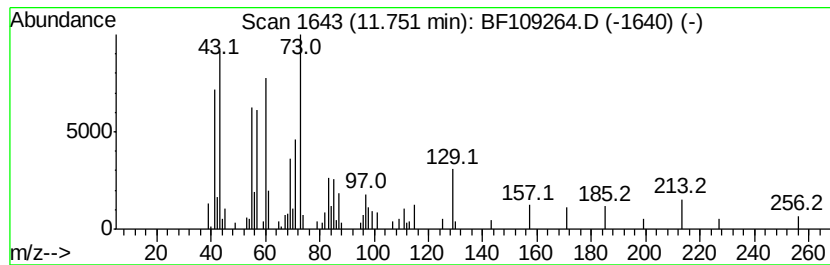
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.75	2.13 ng	96052	Phenanthrene-d10	11.21

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	74
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
4	Tridecanoic acid	214	C13H26O2	000638-53-9	72
5	n-Decanoic acid	172	C10H20O2	000334-48-5	59



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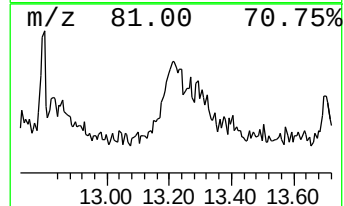
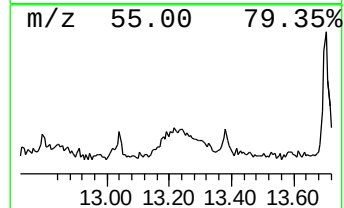
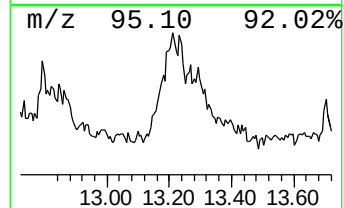
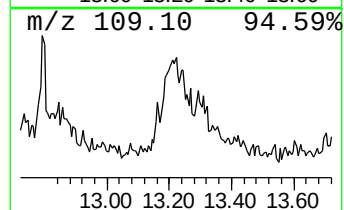
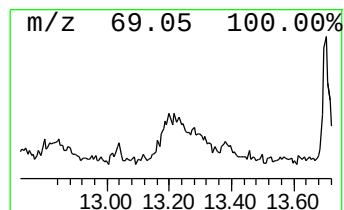
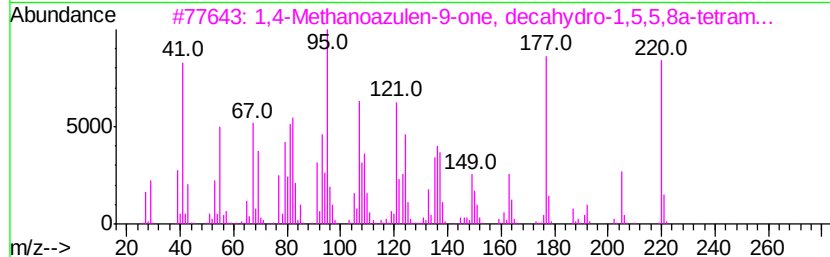
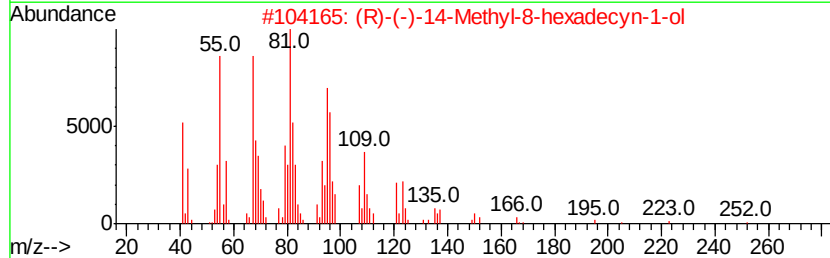
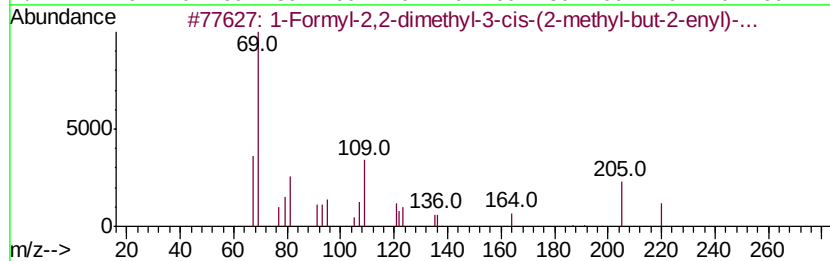
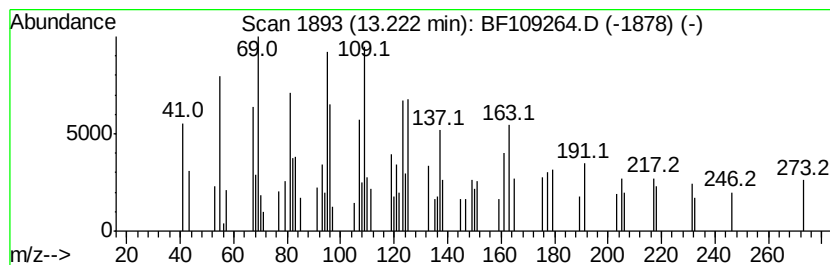
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Peak Number 5 unknown13.22 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.22	3.32 ng	127634	Chrysene-d12	13.83	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Formyl-2,2-dimethyl-3-cis-(2-m...	220	C15H24O	1000144-10-0	42
2	(R)-(-)-14-Methyl-8-hexadecyn-1-ol	252	C17H32O	064566-18-3	41
3	1,4-Methanoazulen-9-one, decahyd...	220	C15H24O	000465-26-9	30
4	1-Formyl-2,2-dimethyl-3-trans-(3...	220	C15H24O	1000144-09-7	25
5	1,E-8,Z-10-Hexadecatriene	220	C16H28	080625-33-8	25



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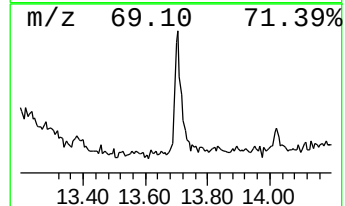
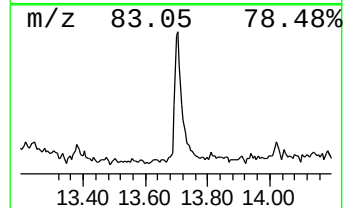
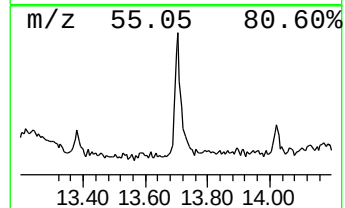
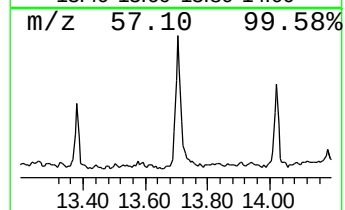
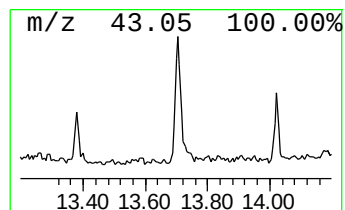
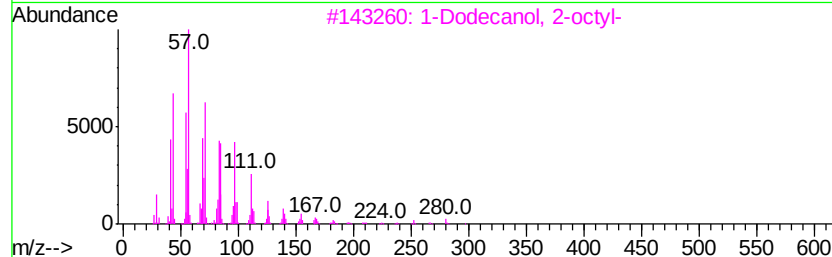
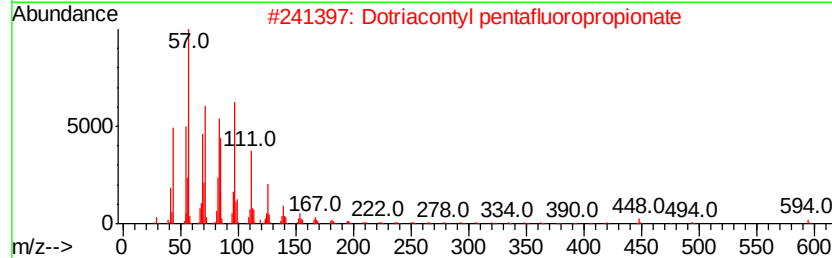
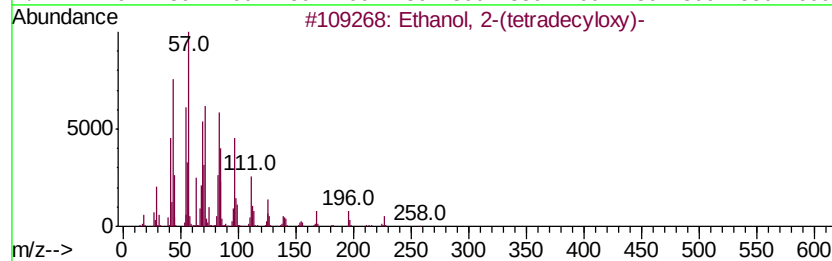
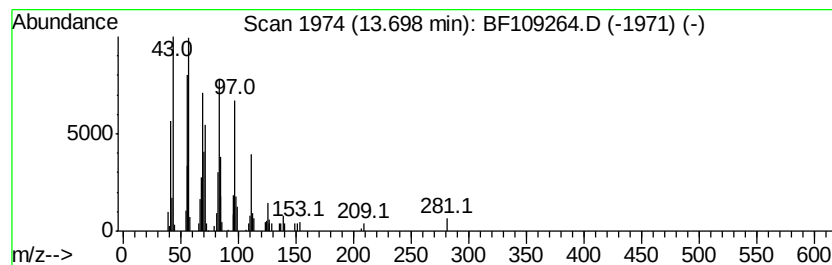
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TIC Integration Parameters: LSCINT.P

Peak Number 6 Ethanol, 2-(tetradecyloxy)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.70	3.75 ng	144300	Chrysene-d12	13.83
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Ethanol, 2-(tetradecyloxy)-	258 C16H34O2	002136-70-1 91
2		Dotriacontyl pentafluoropropionate	612 C35H65F5O2	1000351-81-4 91
3		1-Dodecanol, 2-octyl-	298 C20H42O	005333-42-6 83
4		1-Hexadecanesulfonyl chloride	324 C16H33ClO2S	038775-38-1 83
5		1-Decanol, 2-hexyl-	242 C16H34O	002425-77-6 81



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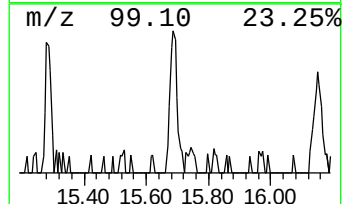
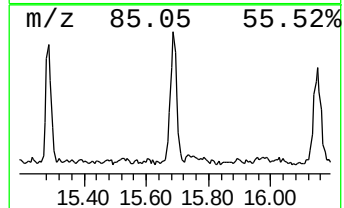
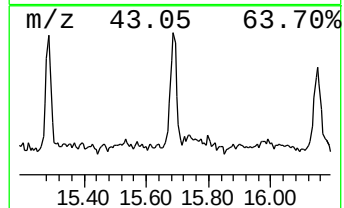
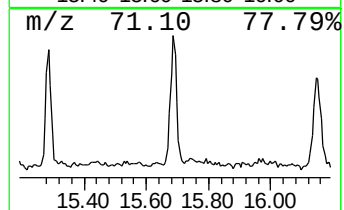
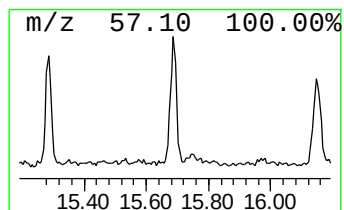
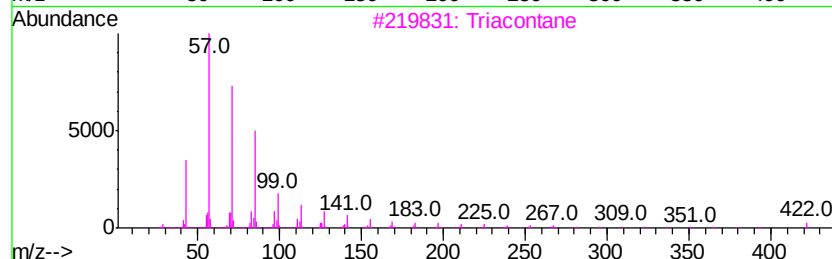
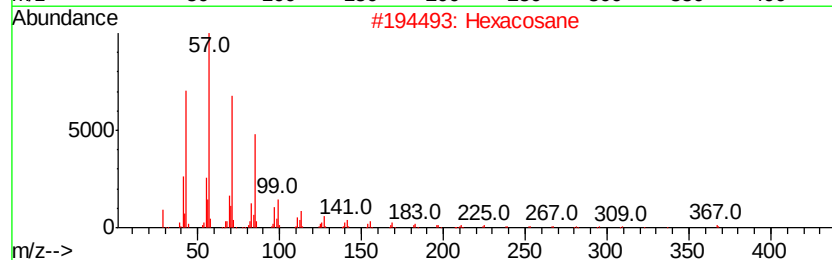
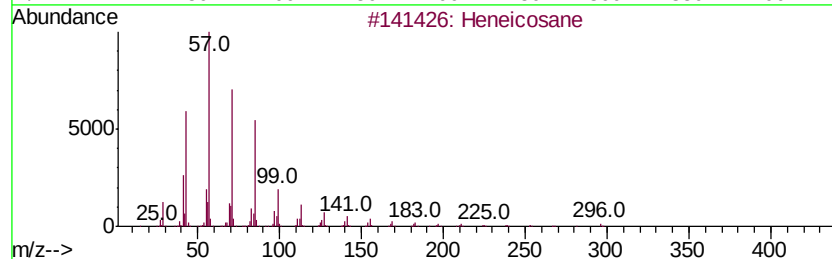
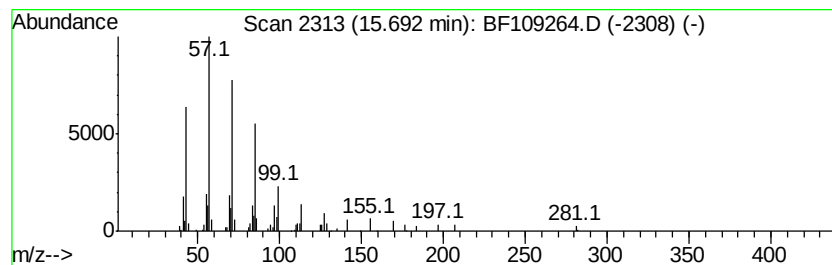
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Heneicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.69	2.47 ng	98905	Perylene-d12	15.24

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane		296	C21H44	000629-94-7	91
2	Hexacosane		366	C26H54	000630-01-3	91
3	triacontane		422	C30H62	000638-68-6	91
4	Eicosane		282	C20H42	000112-95-8	90
5	Octacosane		394	C28H58	000630-02-4	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF092418\
Data File : BF109264.D
Acq On : 24 Sep 2018 13:49
Operator : JU/SJ
Sample : J5023-09
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
NB-PIT-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092218.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...	4.90	5.3	ng	169676	1	6.70	641943	20.0
unknown6.47	6.47	75.4	ng	2418750	1	6.70	641943	20.0
n-Hexadecanoic acid	11.75	2.1	ng	96052	4	11.21	901289	20.0
unknown13.22	13.22	3.3	ng	127634	5	13.83	769162	20.0
Ethanol, 2-(tetra...	13.70	3.8	ng	144300	5	13.83	769162	20.0
Heneicosane	15.69	2.5	ng	98905	6	15.24	800712	20.0