

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF032919\
 Data File : BF113424.D
 Acq On : 29 Mar 2019 20:22
 Operator : JU/SJ
 Sample : K2138-01
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 S6A(2-10)COMP

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-BF032519.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	5.322	545	550	566	rBV	3147702	3541792	71.28%	8.868%
2	6.351	720	725	728	rBV	3288185	3656811	73.60%	9.156%
3	6.475	742	746	751	rBV	3797068	3702903	74.52%	9.272%
4	6.698	781	784	795	rVB	943935	839007	16.89%	2.101%
5	6.857	807	811	826	rBV	3247770	2913680	58.64%	7.296%
6	7.263	876	880	900	rBV	2178217	2470145	49.71%	6.185%
7	7.981	999	1002	1022	rBV	1082769	1079302	21.72%	2.703%
8	9.057	1181	1185	1196	rBV	4282922	4446759	89.50%	11.134%
9	9.145	1197	1200	1210	rVB4	36488	60502	1.22%	0.151%
10	9.451	1249	1252	1257	rBV	257534	245475	4.94%	0.615%
11	9.733	1296	1300	1312	rVB	1276248	1252446	25.21%	3.136%
12	10.386	1406	1411	1417	rBV2	85215	121110	2.44%	0.303%
13	10.522	1429	1434	1441	rBV	2721907	2821813	56.79%	7.066%
14	10.580	1441	1444	1452	rVV	212239	350678	7.06%	0.878%
15	10.639	1452	1454	1464	rVB4	66966	112196	2.26%	0.281%
16	11.086	1523	1530	1533	rBV2	49862	55169	1.11%	0.138%
17	11.210	1547	1551	1559	rBV	1547625	1425665	28.69%	3.570%
18	11.745	1639	1642	1652	rBV3	213473	284960	5.74%	0.714%
19	12.304	1732	1737	1741	rBV2	48537	53577	1.08%	0.134%
20	12.416	1751	1756	1760	rBV	170629	170180	3.43%	0.426%
21	12.527	1772	1775	1785	rBV4	120014	196591	3.96%	0.492%
22	12.610	1785	1789	1792	rVV	219364	205083	4.13%	0.514%
23	12.645	1792	1795	1798	rVB	144449	132957	2.68%	0.333%
24	12.792	1815	1820	1823	rBV	4581835	4968697	100.00%	12.441%
25	12.816	1823	1824	1829	rVB	249340	168595	3.39%	0.422%
26	12.963	1844	1849	1854	rVB4	22775	49886	1.00%	0.125%
27	13.027	1857	1860	1863	rVV	59076	59310	1.19%	0.149%
28	13.333	1909	1912	1915	rBV	87415	81831	1.65%	0.205%
29	13.692	1970	1973	1975	rBV	70130	67687	1.36%	0.169%
30	13.721	1975	1978	1990	rVB6	64779	155618	3.13%	0.390%
31	13.839	1992	1998	2001	rBV	1355431	1506806	30.33%	3.773%
32	14.010	2024	2027	2030	rBV	70719	65623	1.32%	0.164%
33	14.310	2075	2078	2082	rVB	108322	102485	2.06%	0.257%
34	14.604	2125	2128	2133	rBV	151510	132851	2.67%	0.333%

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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:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF032519.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	14.674	2137	2140	2142	rBV	52103	49771	1.00%	0.125%
36	14.845	2165	2169	2177	rBV	138595	241549	4.86%	0.605%
37	14.915	2177	2181	2184	rBV	157437	169776	3.42%	0.425%
38	15.127	2213	2217	2222	rVB	73829	100026	2.01%	0.250%
39	15.180	2223	2226	2231	rVV	55985	74837	1.51%	0.187%
40	15.239	2231	2236	2248	rVB	1043189	1484356	29.87%	3.717%
41	15.656	2303	2307	2313	rBV	126358	181324	3.65%	0.454%
42	16.115	2381	2385	2393	rVB2	78631	137026	2.76%	0.343%

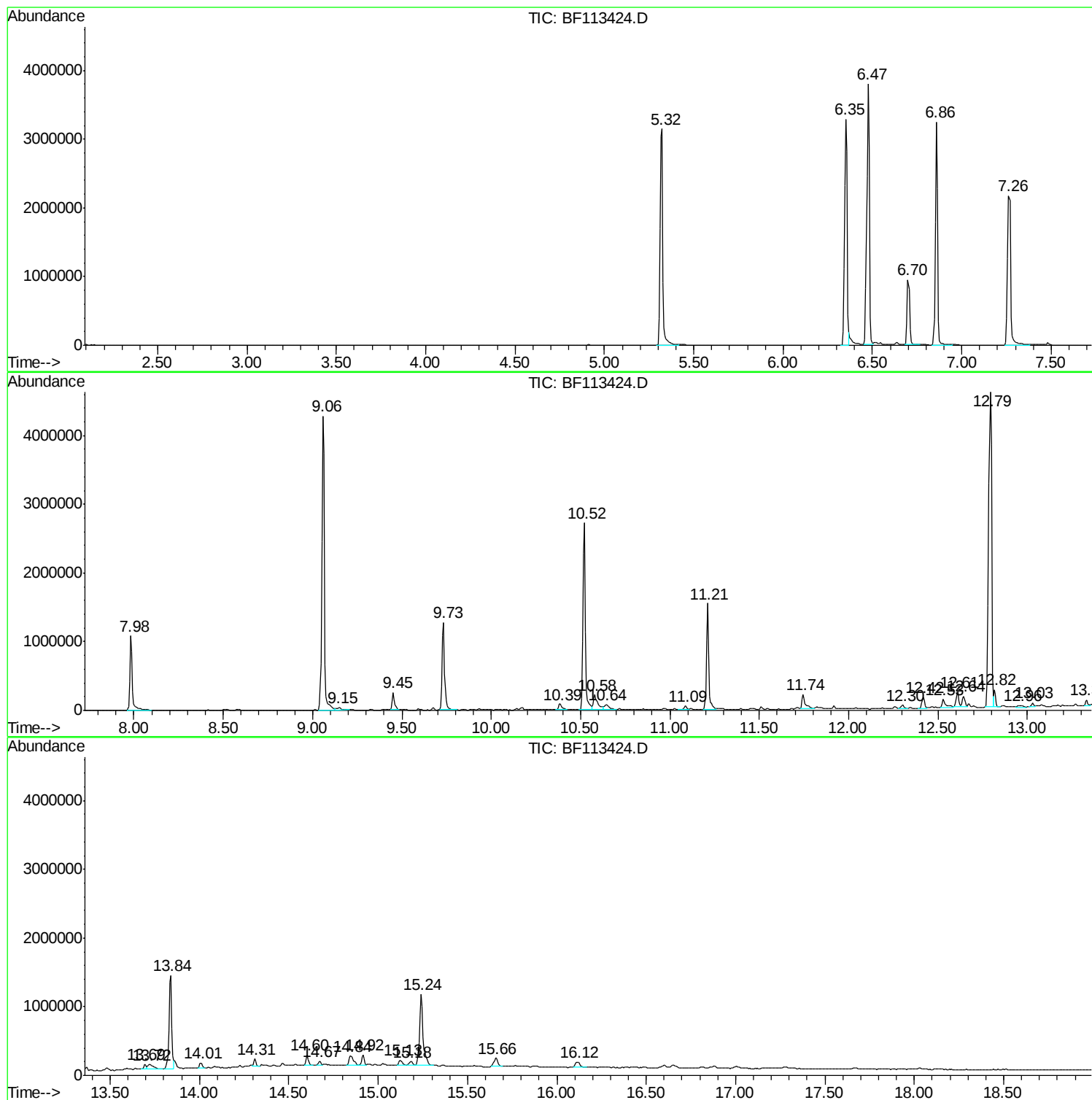
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ClientSampled :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF032519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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S6A(2-10)COMP

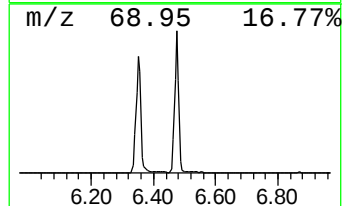
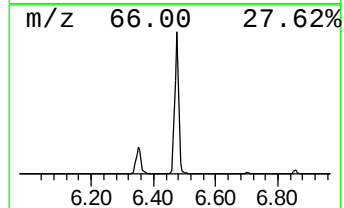
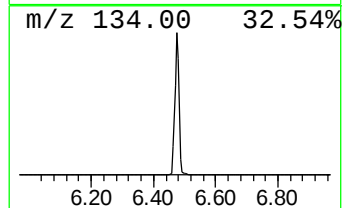
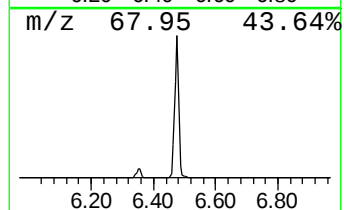
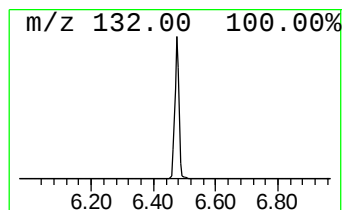
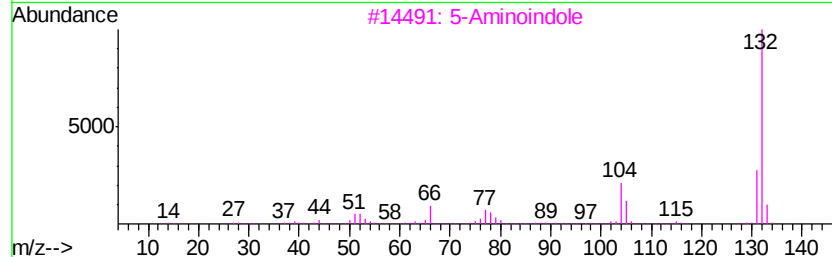
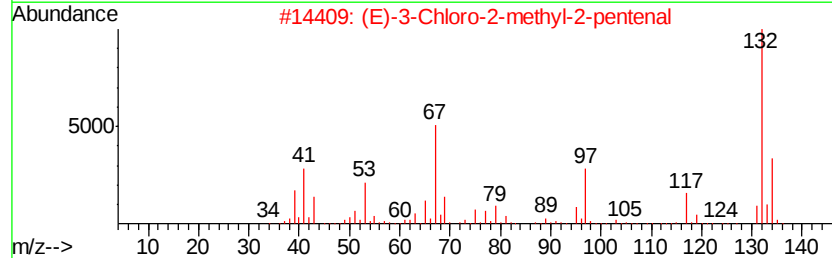
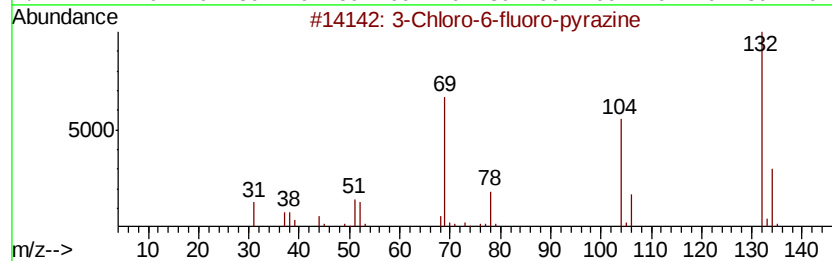
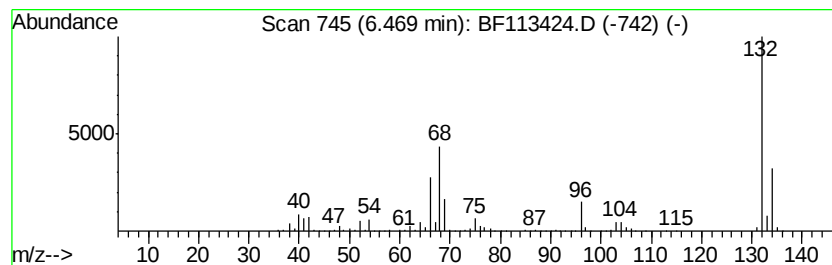
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 unknown6.47 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.47	88.27 ng	3702900	1,4-Dichlorobenzene-d4	6.70

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
5		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9



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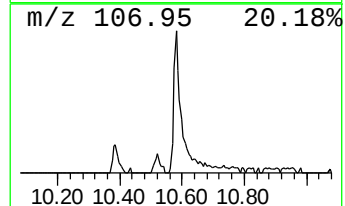
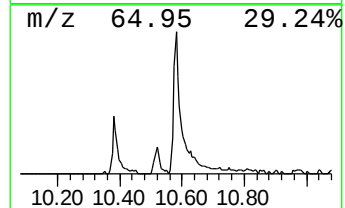
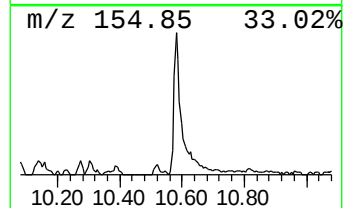
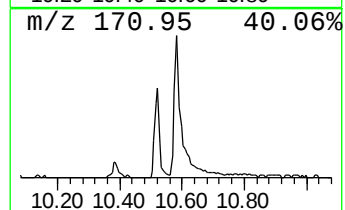
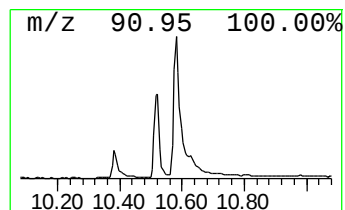
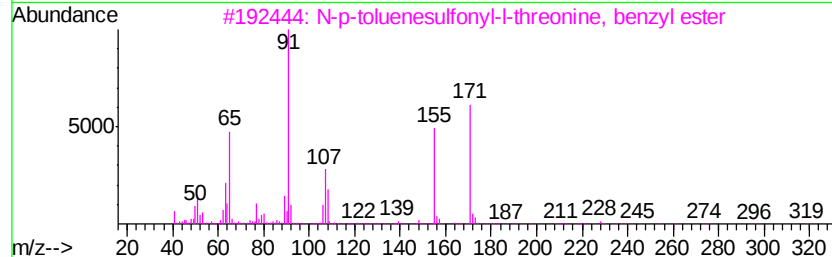
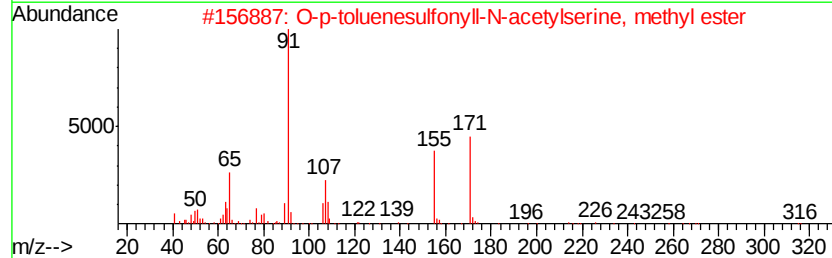
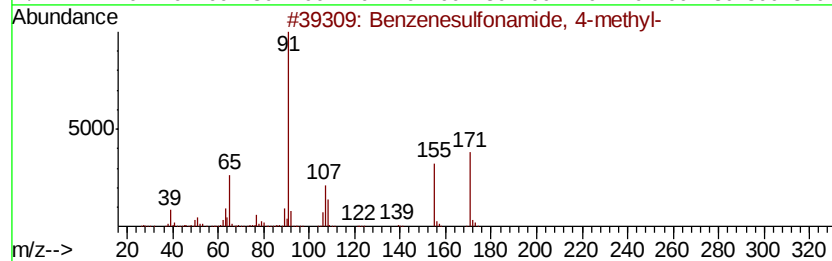
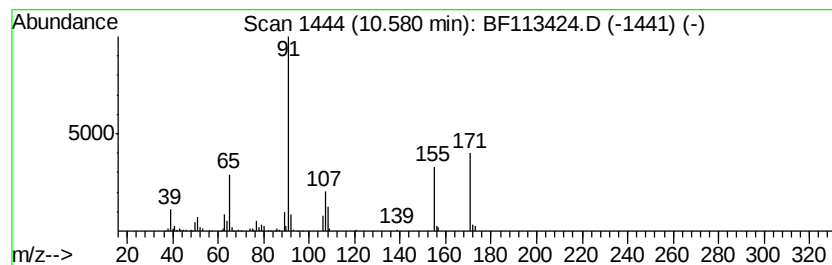
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Peak Number 3 Benzenesulfonamide, 4-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD		R.T.	
10.58	4.92 ng	350678	Phenanthrene-d10		11.21	
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Benzenesulfonamide, 4-methyl-	171	C7H9NO2S	000070-55-3	98
2		O-p-toluenesulfonyll-N-acetylser...	315	C13H17NO6S	1000126-44-8	90
3		N-p-toluenesulfonyl-l-threonine,...	363	C18H21NO5S	1000130-34-4	72
4		Pyridine-2-carbonitrile, 3,5,6-t...	375	C13H8Cl3N3O2S	255713-77-0	35
5		N-carbobenzyloxy-cysteine	255	C11H13NO4S	1000131-22-5	27



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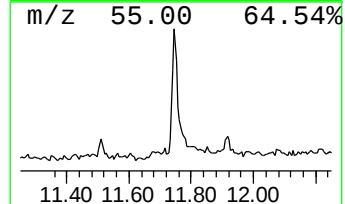
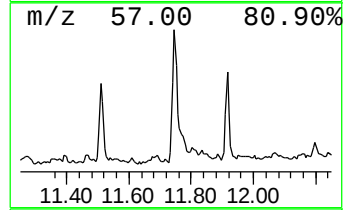
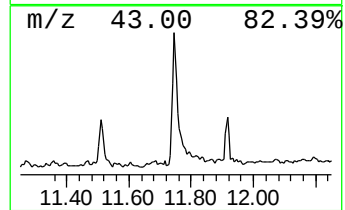
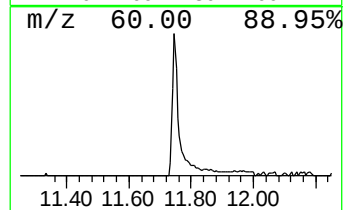
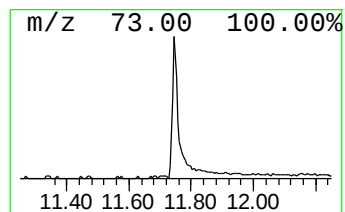
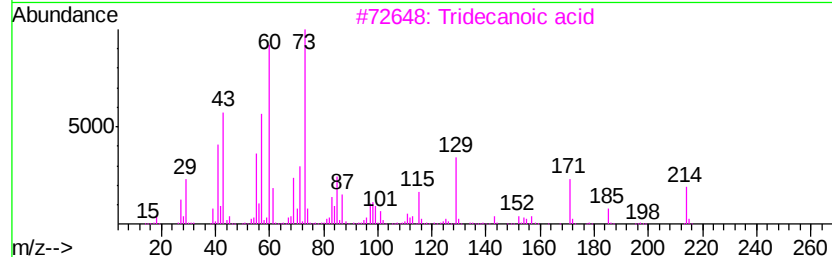
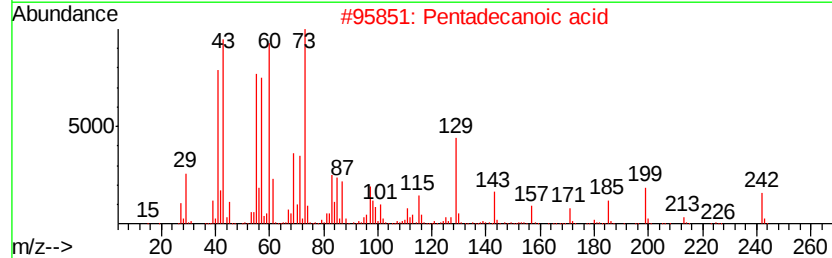
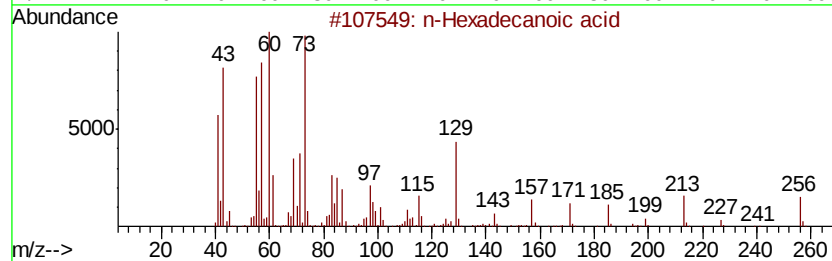
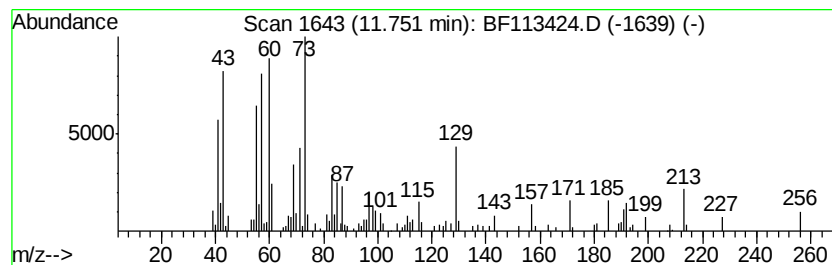
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.75	4.00 ng	284960	Phenanthrene-d10	11.21

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	91
3		Tridecanoic acid	214	C13H26O2	000638-53-9	81
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5		n-Decanoic acid	172	C10H20O2	000334-48-5	62



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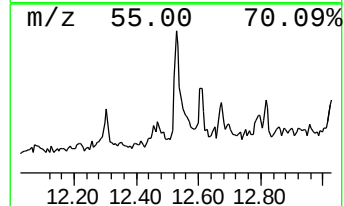
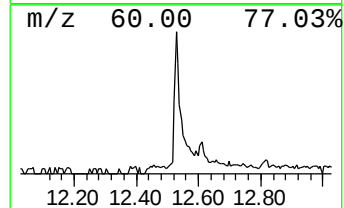
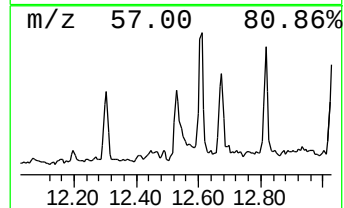
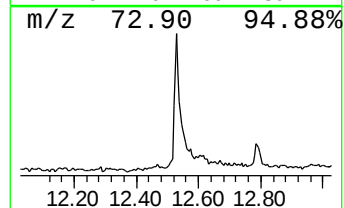
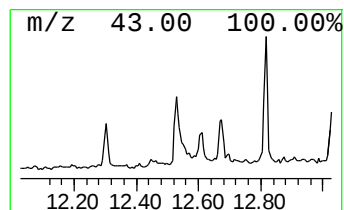
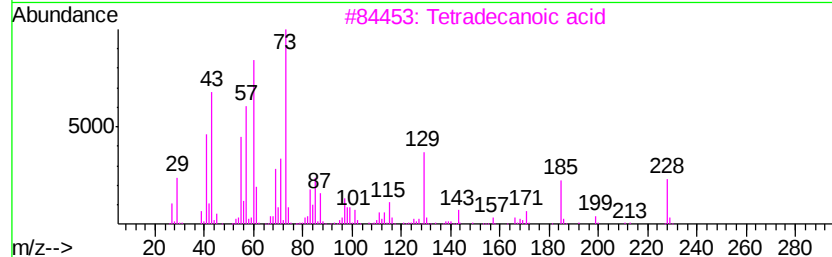
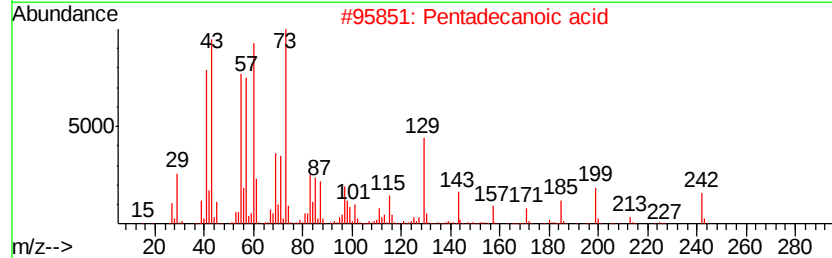
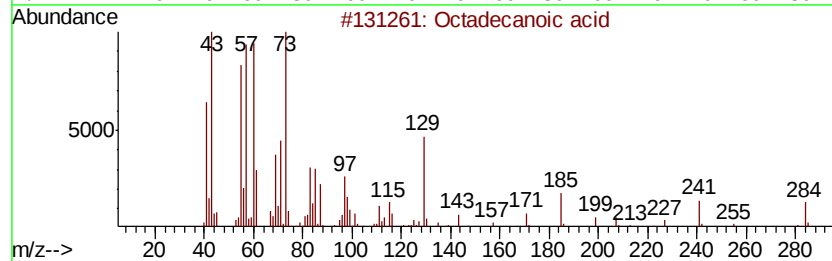
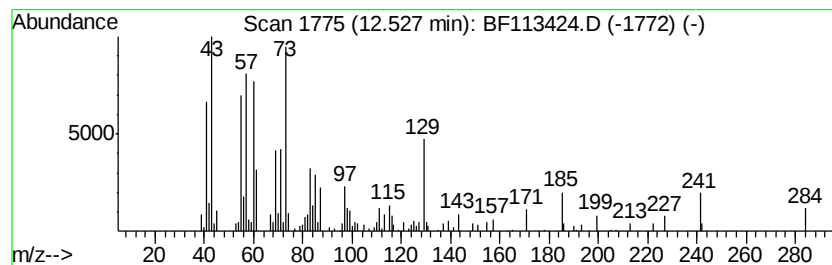
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.53	2.61 ng	196591	Chrysene-d12	13.84

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	87
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	72
4		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	46
5		Oxalic acid, propyl tetradecyl e...	328	C19H36O4	1000309-26-7	30



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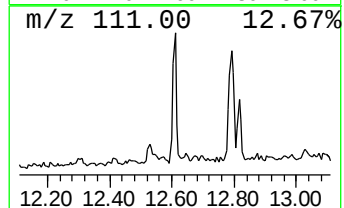
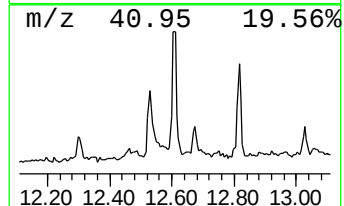
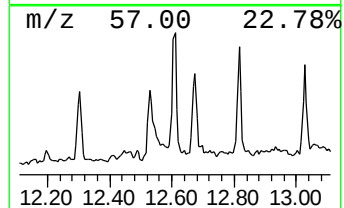
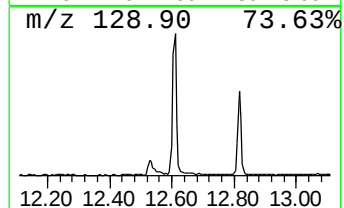
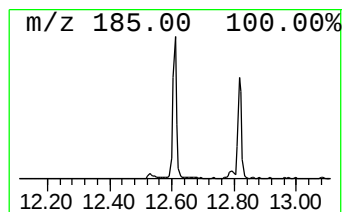
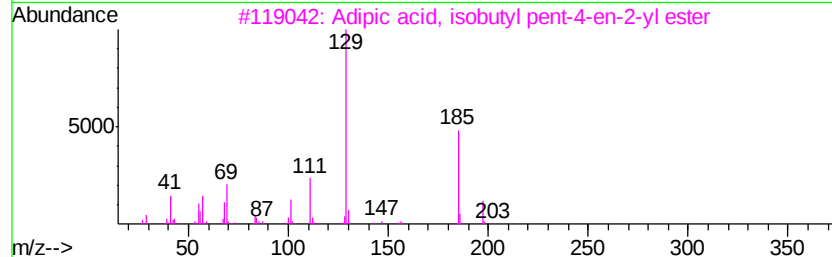
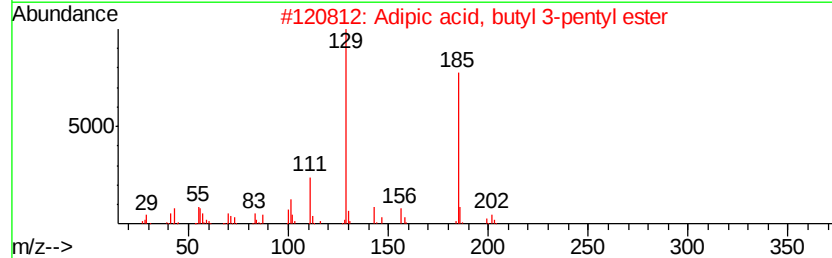
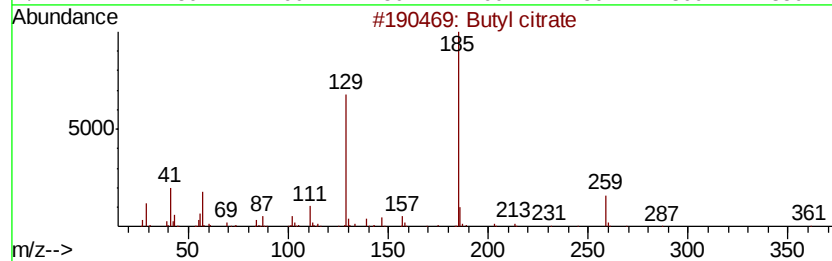
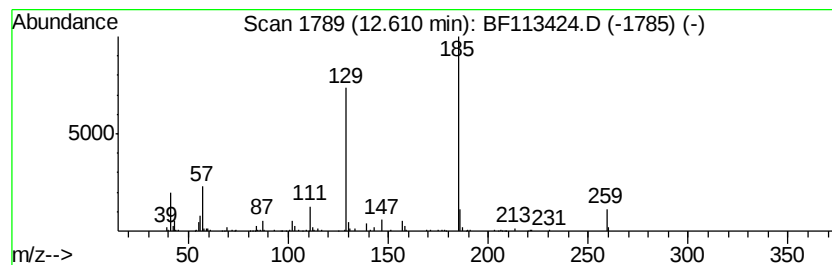
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF032519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Butyl citrate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.61	2.72 ng	205083	Chrysene-d12	13.84
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Butyl citrate	360 C18H32O7	000077-94-1	91
2	Adipic acid, butyl 3-pentyl ester	272 C15H28O4	1000324-60-5	78
3	Adipic acid, isobutyl pent-4-en-...	270 C15H26O4	1000354-11-8	72
4	Adipic acid, butyl 2-methylpent-...	286 C16H30O4	1000353-55-8	72
5	Adipic acid, 2,4-dimethylpent-3-...	300 C17H32O4	1000349-77-6	64



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF032919\
Data File : BF113424.D
Acq On : 29 Mar 2019 20:22
Operator : JU/SJ
Sample : K2138-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S6A(2-10)COMP

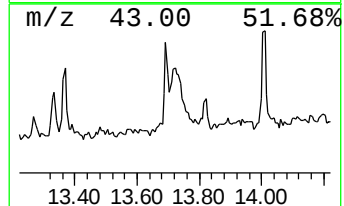
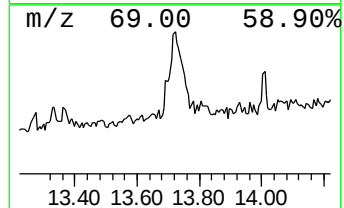
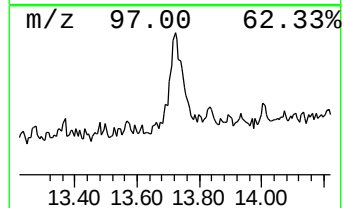
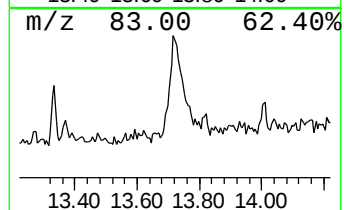
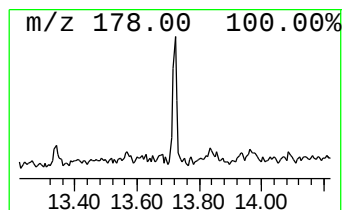
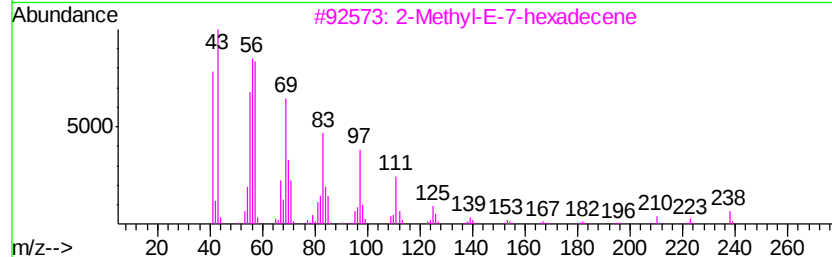
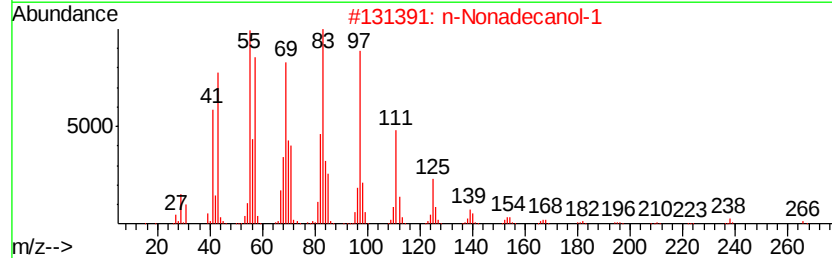
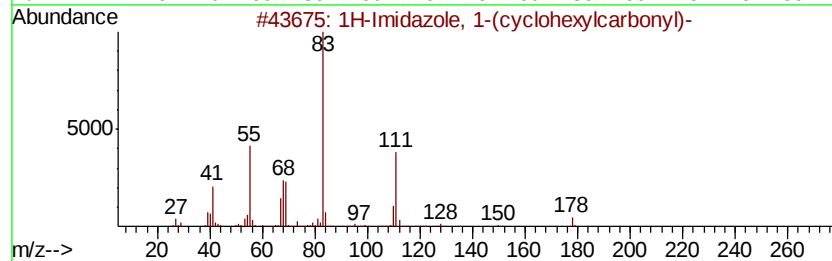
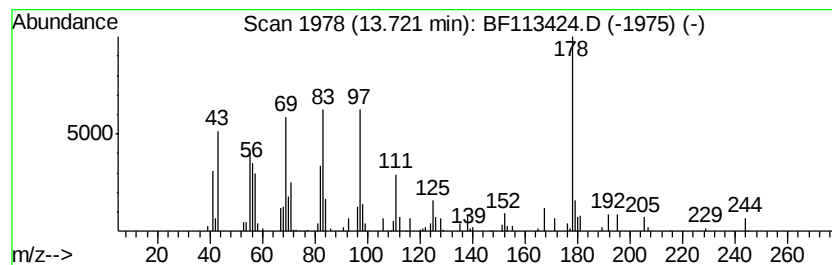
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown13.72 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.72	2.07 ng	155618	Chrysene-d12	13.84

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1H-Imidazole, 1-(cyclohexylcarbo...	178	C10H14N2O	060718-45-8	38
2		n-Nonadecanol-1	284	C19H40O	001454-84-8	27
3		2-Methyl-E-7-hexadecene	238	C17H34	064183-52-4	27
4		2-Benzothiazolamine, 5,6-dimethyl-	178	C9H10N2S	029927-08-0	25
5		Heptacosyl acetate	438	C29H58O2	1000351-78-2	22



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF032919\
Data File : BF113424.D
Acq On : 29 Mar 2019 20:22
Operator : JU/SJ
Sample : K2138-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S6A(2-10)COMP

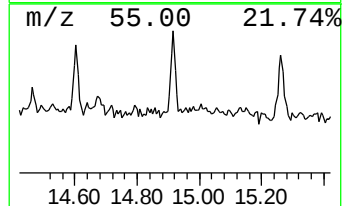
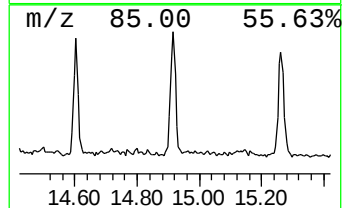
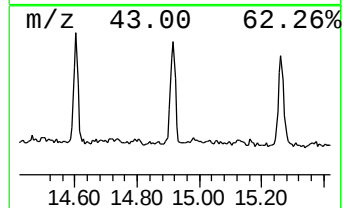
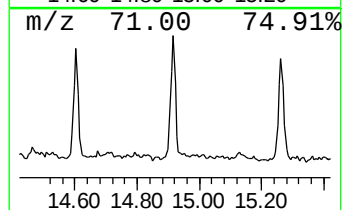
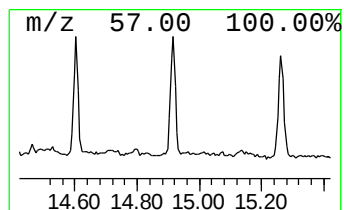
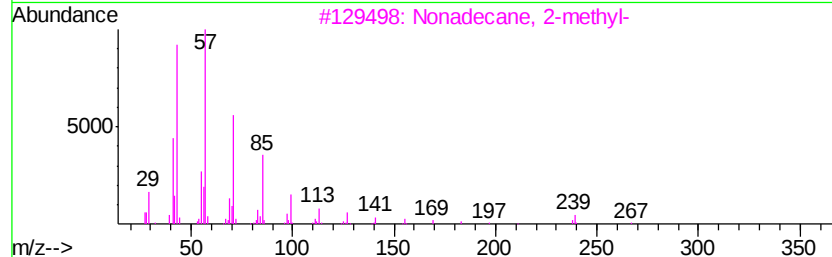
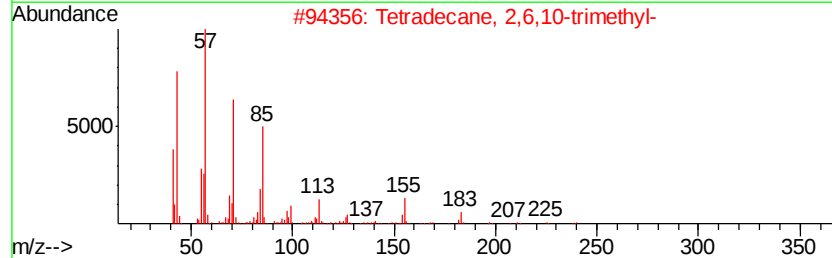
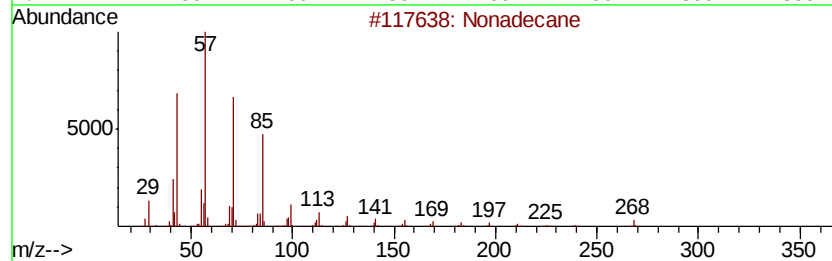
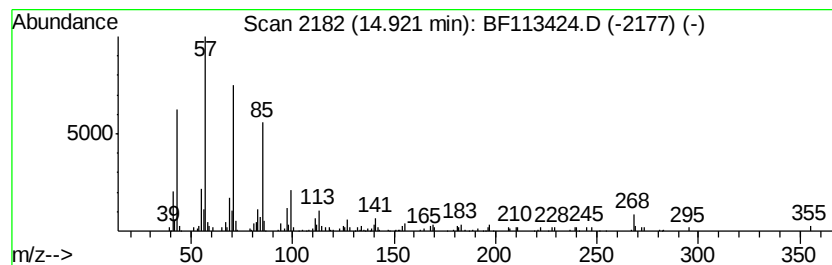
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Nonadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.92	2.29 ng	169776	Perylene-d12	15.24

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane		268	C19H40	000629-92-5	95
2	Tetradecane, 2,6,10-trimethyl-		240	C17H36	014905-56-7	90
3	Nonadecane, 2-methyl-		282	C20H42	001560-86-7	87
4	Octacosane		394	C28H58	000630-02-4	87
5	Heneicosane		296	C21H44	000629-94-7	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF032919\
Data File : BF113424.D
Acq On : 29 Mar 2019 20:22
Operator : JU/SJ
Sample : K2138-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S6A(2-10)COMP

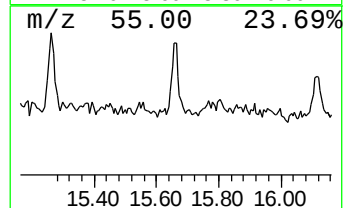
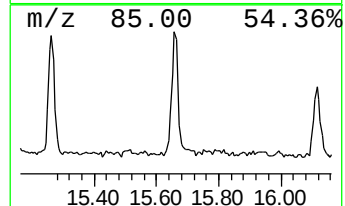
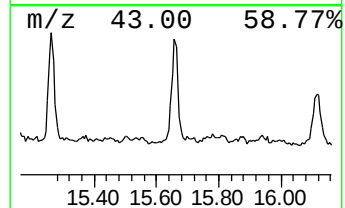
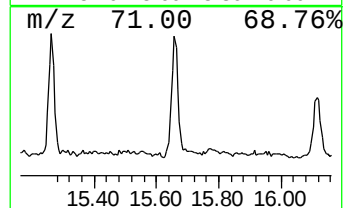
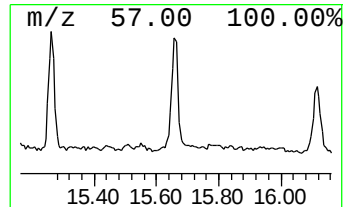
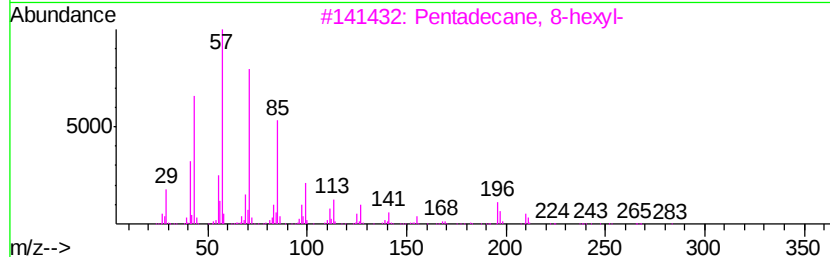
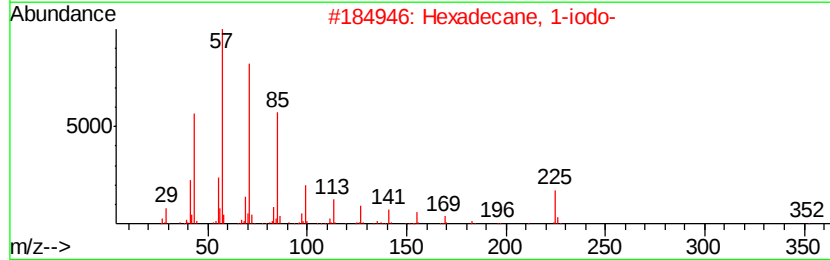
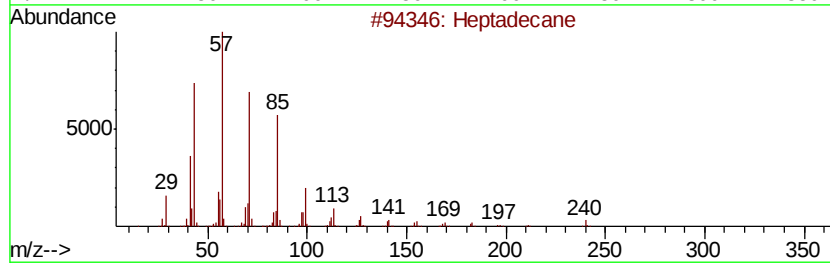
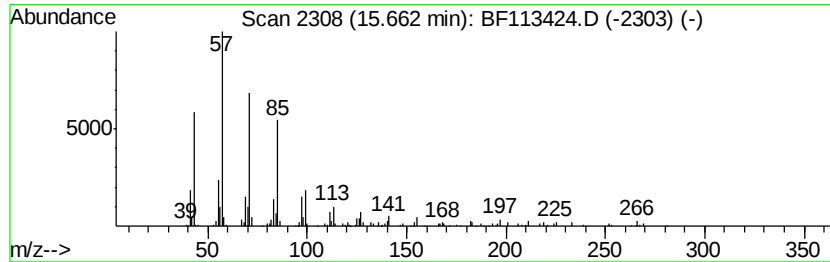
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Heptadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.66	2.44 ng	181324	Perylene-d12	15.24

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane		240	C17H36	000629-78-7	87
2	Hexadecane, 1-iodo-		352	C16H33I	000544-77-4	86
3	Pentadecane, 8-hexyl-		296	C21H44	013475-75-7	86
4	Octacosane		394	C28H58	000630-02-4	83
5	Octadecane, 1-iodo-		380	C18H37I	000629-93-6	80



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Sample : K2138-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S6A(2-10)COMP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF032519.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
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Benzenesulfonamid...	10.58	4.9	ng	350678	4	11.21	1425670	20.0
n-Hexadecanoic acid	11.75	4.0	ng	284960	4	11.21	1425670	20.0
Octadecanoic acid	12.53	2.6	ng	196591	5	13.84	1506810	20.0
Butyl citrate	12.61	2.7	ng	205083	5	13.84	1506810	20.0
unknown13.72	13.72	2.1	ng	155618	5	13.84	1506810	20.0
Nonadecane	14.92	2.3	ng	169776	6	15.24	1484360	20.0
Heptadecane	15.66	2.4	ng	181324	6	15.24	1484360	20.0