

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF010719\
 Data File : BF111899.D
 Acq On : 8 Jan 2019 1:36
 Operator : JU/SJ
 Sample : K1044-02 5X
 Misc :
 ALS Vial : 23 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 CPSB-08(20-25)

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-BF010719.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	2.152	7	11	14	rBV2	19958	24929	3.40%	0.284%
2	5.093	508	511	521	rVB	25967	27646	3.77%	0.314%
3	5.522	580	584	595	rVB	486566	450322	61.41%	5.121%
4	6.528	751	755	764	rBV	509197	470901	64.21%	5.355%
5	6.663	774	778	785	rBV	576070	459289	62.63%	5.223%
6	6.887	813	816	820	rBV	733671	662269	90.31%	7.532%
7	7.045	839	843	847	rBV	469626	368546	50.26%	4.191%
8	7.298	881	886	895	rBV	53078	55433	7.56%	0.630%
9	7.445	907	911	918	rBV	264303	248759	33.92%	2.829%
10	8.169	1031	1034	1038	rBV	766520	717766	97.88%	8.163%
11	9.245	1213	1217	1224	rBV	530006	435246	59.35%	4.950%
12	9.633	1281	1283	1290	rVB	44011	39385	5.37%	0.448%
13	9.928	1329	1333	1337	rBV	865798	725089	98.88%	8.246%
14	10.716	1463	1467	1471	rBV	321745	275945	37.63%	3.138%
15	10.792	1476	1480	1483	rVB	105431	88071	12.01%	1.002%
16	11.310	1566	1568	1570	rVB	13970	10826	1.48%	0.123%
17	11.416	1582	1586	1589	rBV	811838	705142	96.16%	8.019%
18	11.439	1589	1590	1593	rVV	40141	32233	4.40%	0.367%
19	11.469	1593	1595	1601	rVB4	19587	20849	2.84%	0.237%
20	11.545	1603	1608	1613	rBV4	10327	13492	1.84%	0.153%
21	11.627	1619	1622	1625	rBV2	19153	18107	2.47%	0.206%
22	11.798	1649	1651	1654	rBV3	8466	9117	1.24%	0.104%
23	11.933	1669	1674	1679	rBV2	36688	43781	5.97%	0.498%
24	12.486	1766	1768	1770	rBV2	23891	20240	2.76%	0.230%
25	12.510	1770	1772	1774	rVB	39566	31224	4.26%	0.355%
26	12.627	1790	1792	1796	rBV4	10383	14830	2.02%	0.169%
27	12.780	1816	1818	1821	rBV3	11654	10201	1.39%	0.116%
28	12.992	1849	1854	1858	rBV	550255	476812	65.02%	5.422%
29	13.180	1884	1886	1888	rBV3	13969	13687	1.87%	0.156%
30	13.227	1892	1894	1898	rVV5	15034	18590	2.54%	0.211%
31	13.274	1900	1902	1905	rVV4	10670	11204	1.53%	0.127%
32	13.392	1919	1922	1924	rBV4	12317	17314	2.36%	0.197%
33	13.545	1945	1948	1951	rBV4	25670	41903	5.71%	0.477%
34	13.686	1966	1972	1978	rBV3	83775	149691	20.41%	1.702%

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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

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Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	13.815	1992	1994	2003	rVB10	27702	60999	8.32%	0.694%
36	13.898	2003	2008	2011	rBV2	87431	141760	19.33%	1.612%
37	14.051	2031	2034	2038	rBV	776962	733323	100.00%	8.340%
38	14.139	2047	2049	2050	rBV2	35952	24872	3.39%	0.283%
39	14.333	2080	2082	2086	rBV	104577	95490	13.02%	1.086%
40	14.521	2111	2114	2120	rBV	70049	97373	13.28%	1.107%
41	14.974	2188	2191	2198	rVB3	91658	141627	19.31%	1.611%
42	15.174	2222	2225	2228	rVB	82640	84190	11.48%	0.957%
43	15.315	2247	2249	2253	rBV5	42085	67624	9.22%	0.769%
44	15.539	2282	2287	2295	rVB	471857	637150	86.89%	7.246%

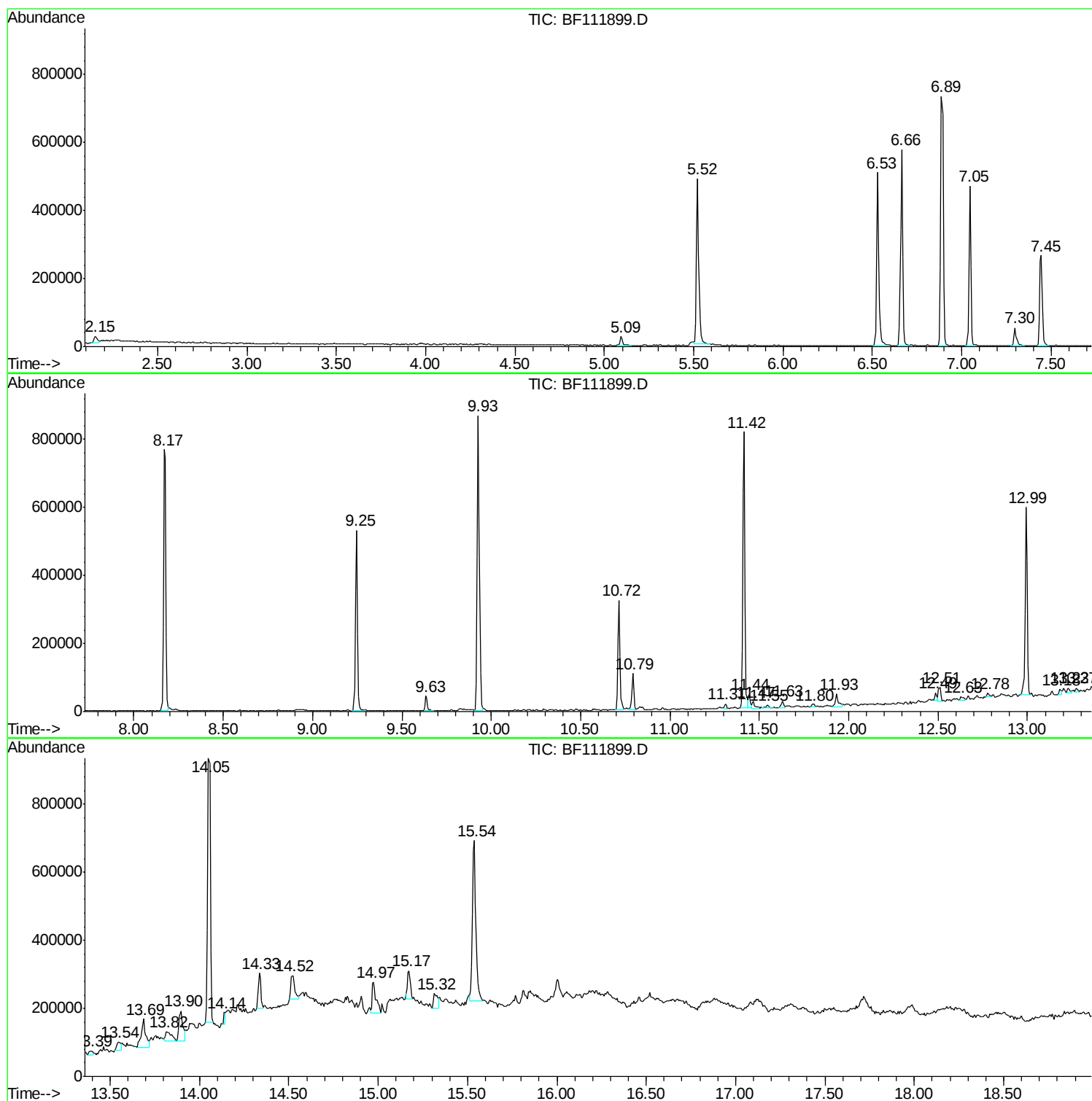
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF010719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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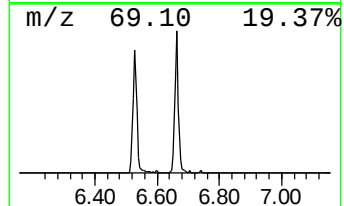
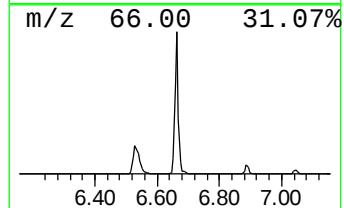
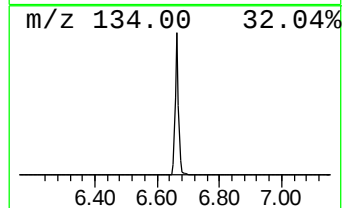
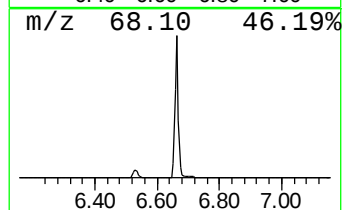
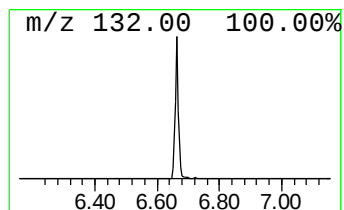
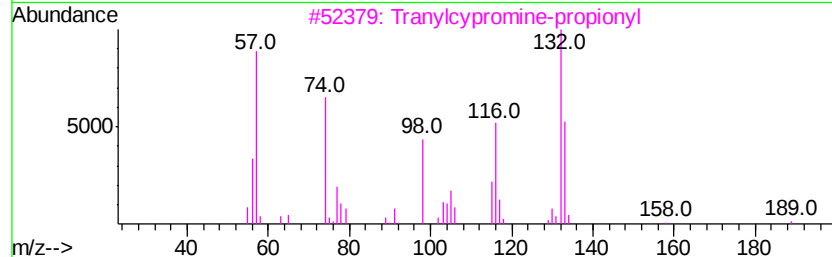
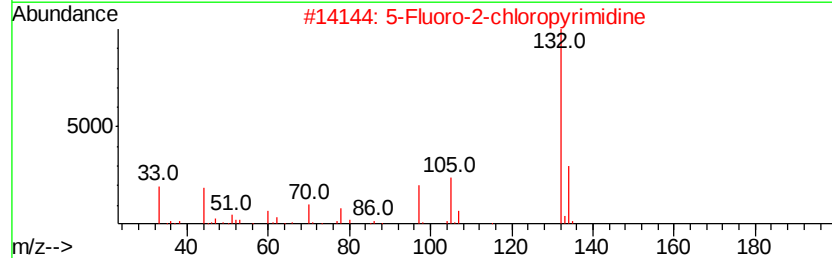
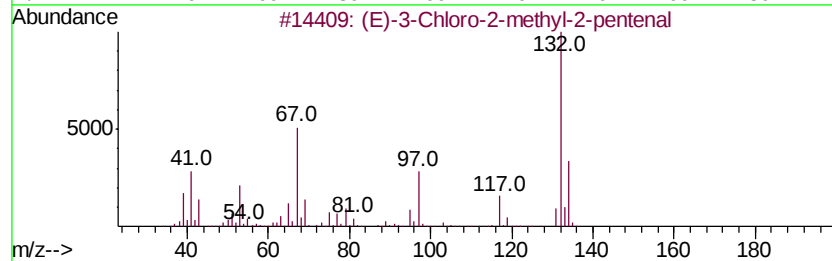
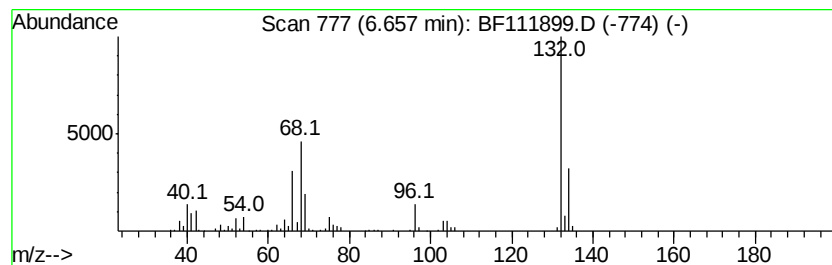
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF010719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown6.66 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.66	13.87 ng	459289	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	17
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
3		Tranvlcyproline-propionyl	189	C12H15NO	1000123-86-3	10
4		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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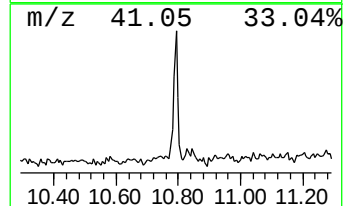
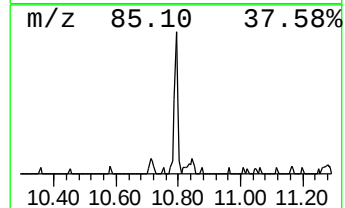
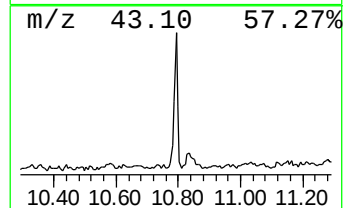
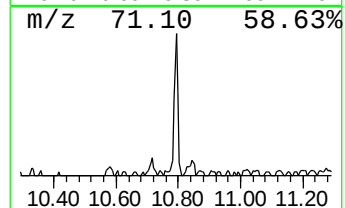
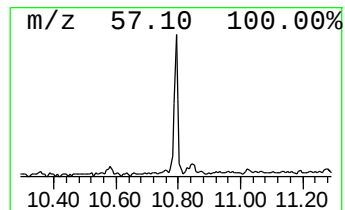
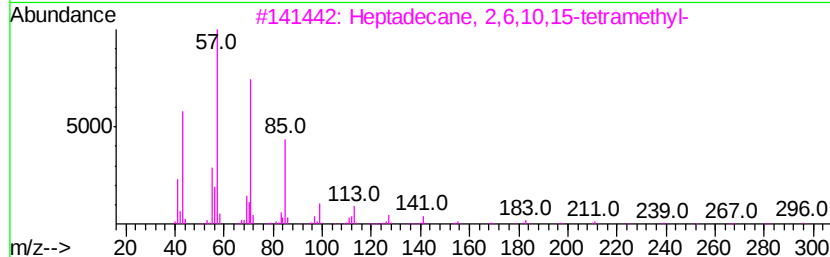
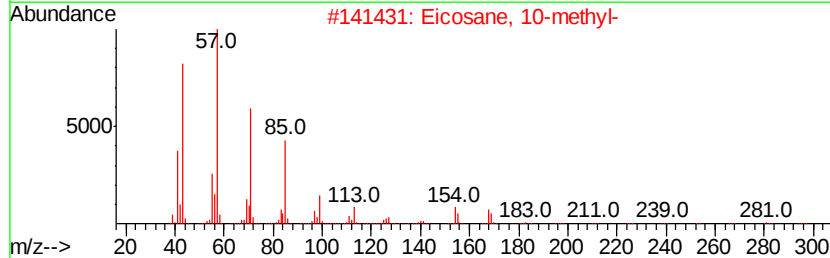
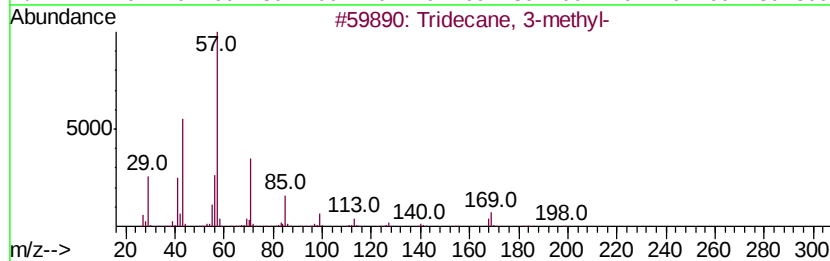
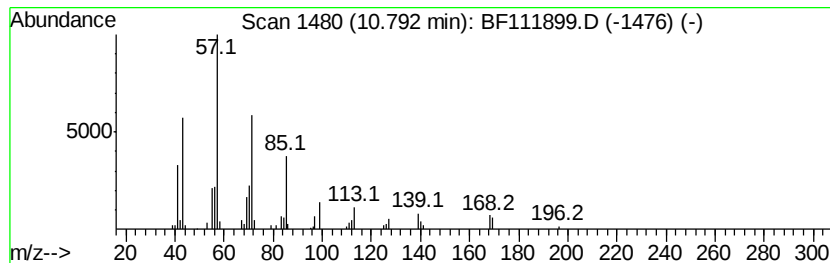
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Tridecane, 3-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.79	2.50 ng	88071	Phenanthrene-d10	11.42	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane, 3-methyl-	198	C14H30	006418-41-3	80
2	Eicosane, 10-methyl-	296	C21H44	054833-23-7	72
3	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	72
4	Pentadecane, 2,6,10-trimethyl-	254	C18H38	003892-00-0	64
5	10-Methylnonadecane	282	C20H42	056862-62-5	64



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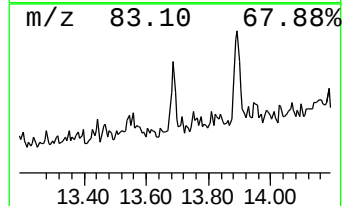
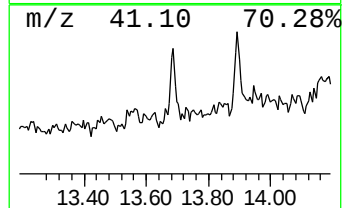
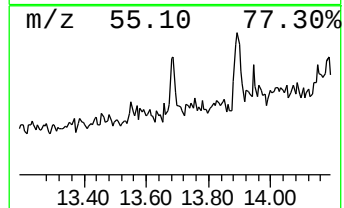
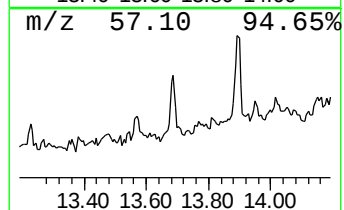
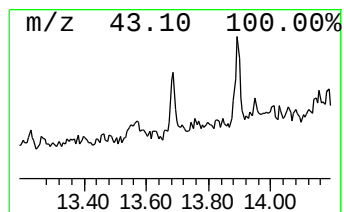
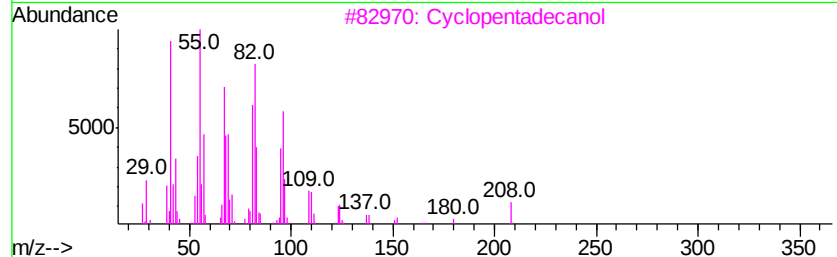
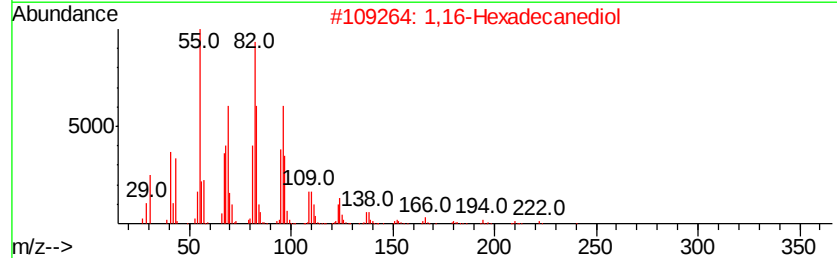
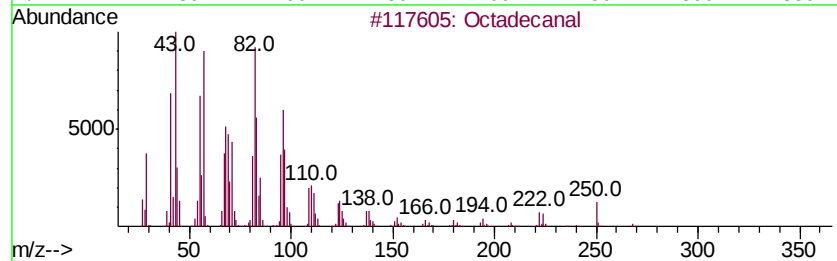
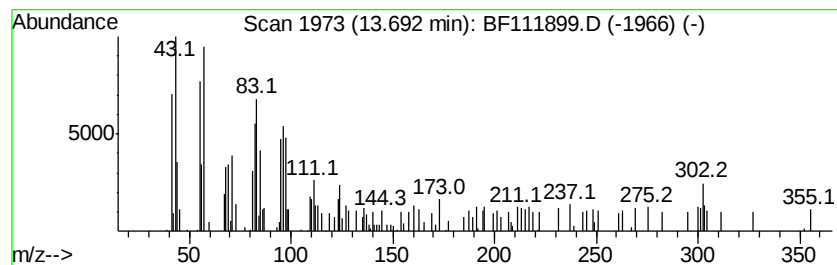
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Octadecanal Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.69	4.08 ng	149691	Chrysene-d12	14.06	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanal	268	C18H36O	000638-66-4	80
2	1,16-Hexadecanediol	258	C16H34O2	007735-42-4	62
3	Cyclopentadecanol	226	C15H30O	004727-17-7	49
4	Dodecane, 5-cyclohexyl-	252	C18H36	013151-85-4	46
5	7-Azabicyclo[4.1.0]heptane, 1-me...	111	C7H13N	025022-25-7	38



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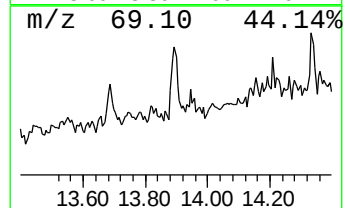
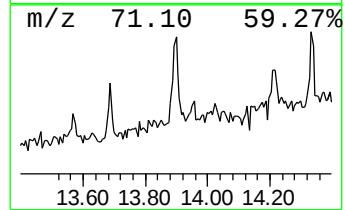
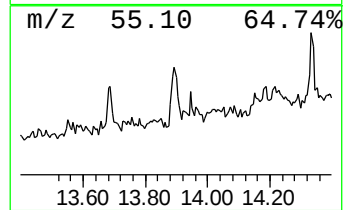
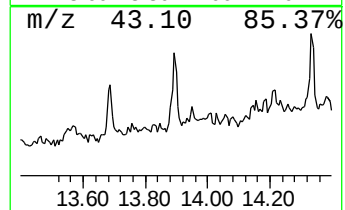
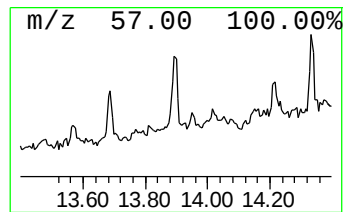
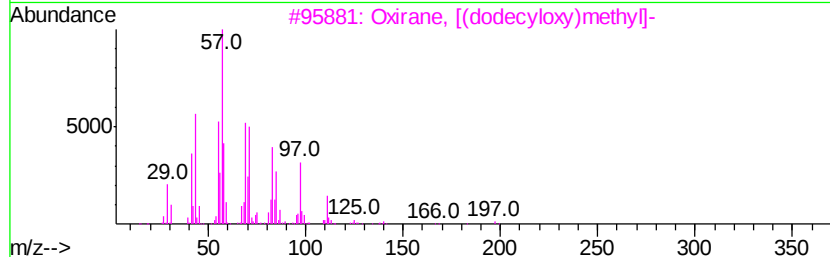
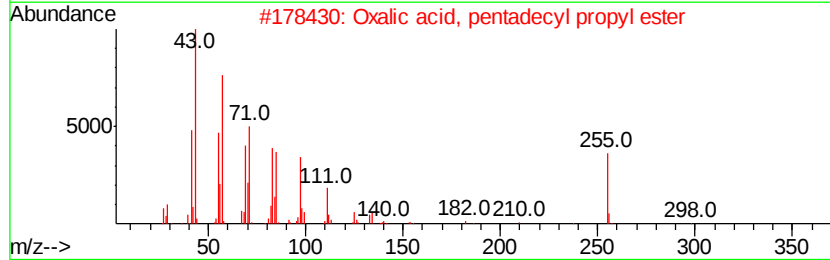
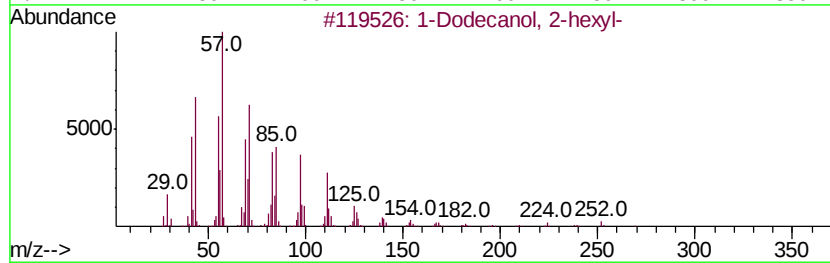
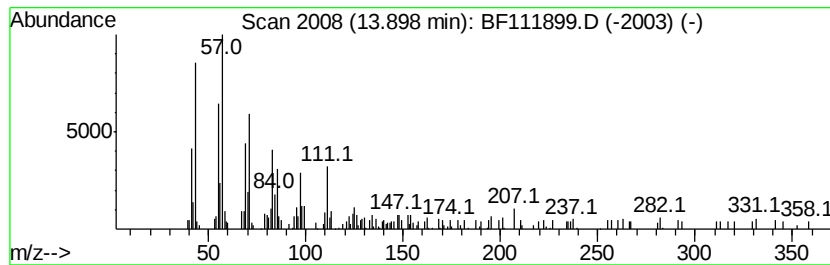
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 1-Dodecanol, 2-hexyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.		
13.90	3.87 ng	141760	Chrysene-d12	14.06		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Dodecanol, 2-hexyl-	270	C18H38O	110225-00-8	83
2		Oxalic acid, pentadecyl propyl e...	342	C20H38O4	1000309-26-8	64
3		Oxirane, [(dodecyloxy)methyl]-	242	C15H30O2	002461-18-9	64
4		1-Decanol, 2-octyl-	270	C18H38O	045235-48-1	64
5		Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	53



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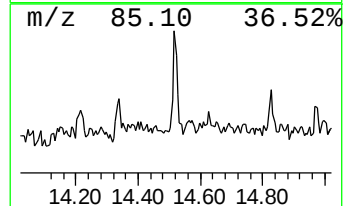
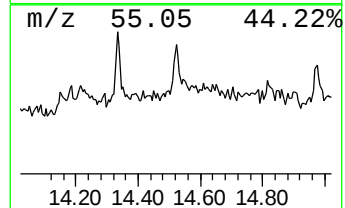
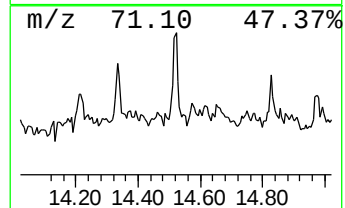
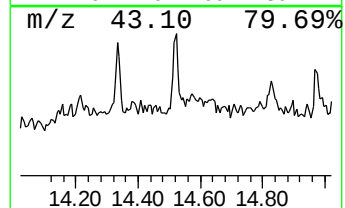
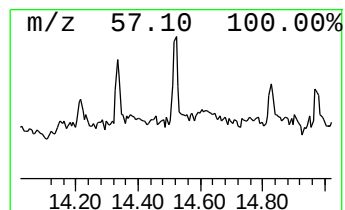
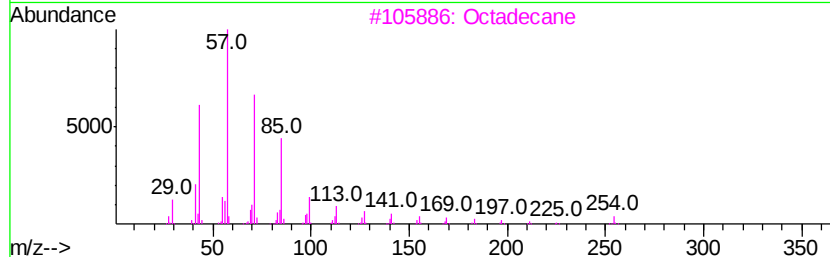
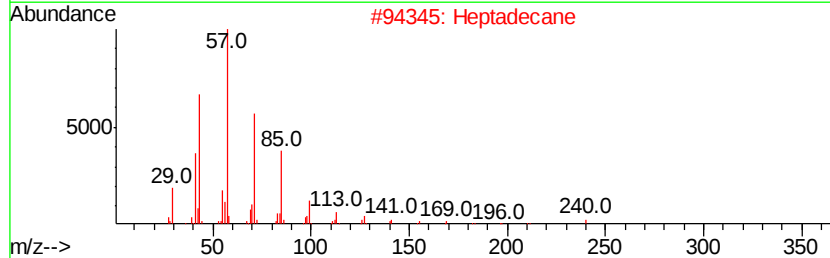
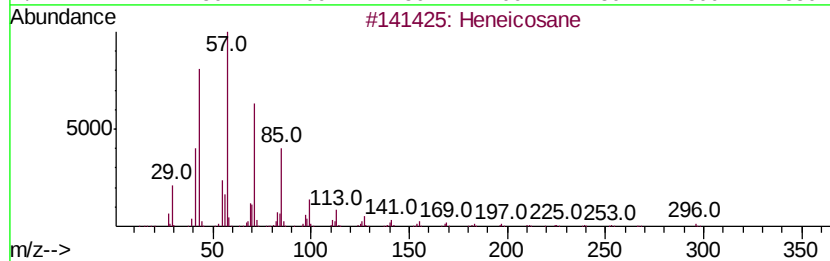
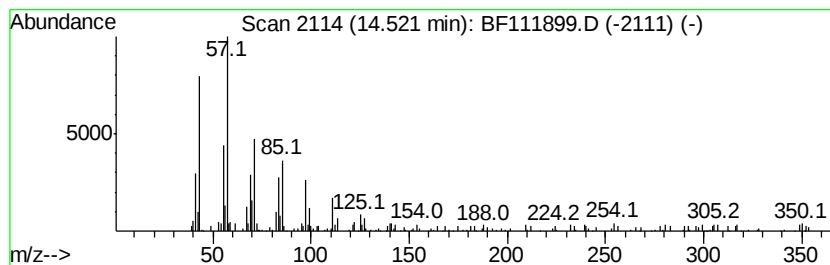
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BNA_F
ClientSampleId :
CPSB-08(20-25)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF010719.M
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.
14.52	2.66 ng	97373	Chrysene-d12		14.06
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	90
2	Heptadecane	240	C17H36	000629-78-7	90
3	Octadecane	254	C18H38	000593-45-3	89
4	Sulfurous acid, octadecyl 2-prop...	376	C21H44O3S	1000309-12-7	68
5	Pentadecane	212	C15H32	000629-62-9	64



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF010719\
Data File : BF111899.D
Acq On : 8 Jan 2019 1:36
Operator : JU/SJ
Sample : K1044-02 5X
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CPSB-08(20-25)

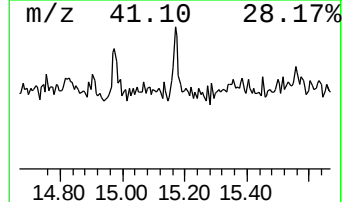
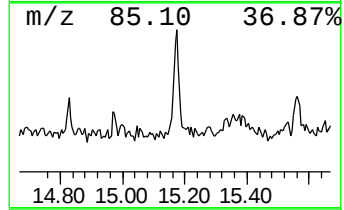
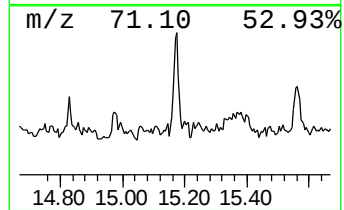
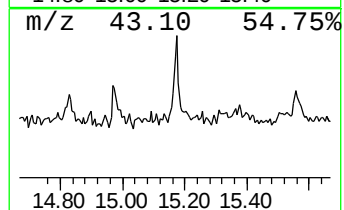
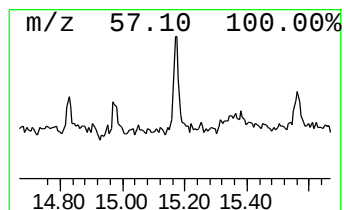
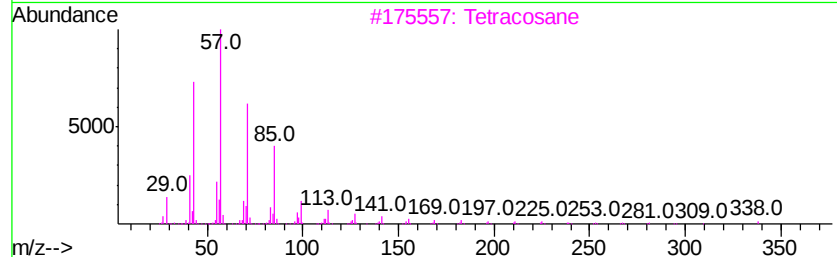
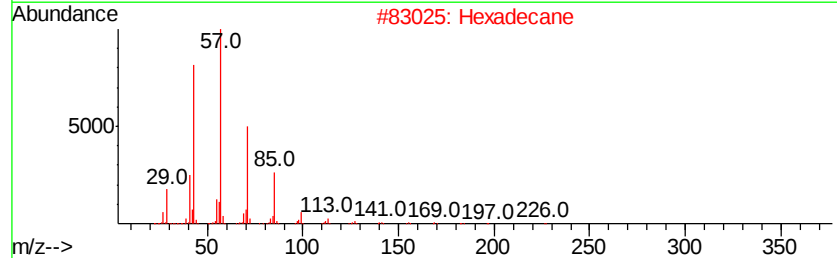
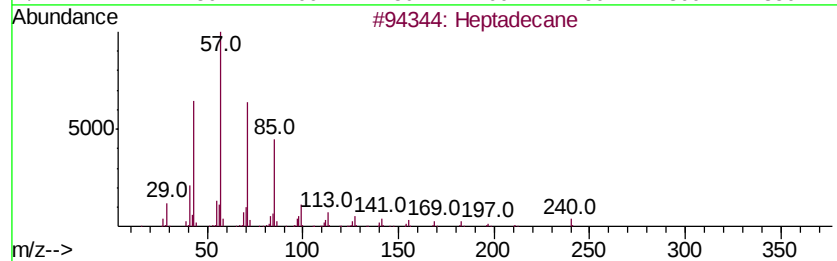
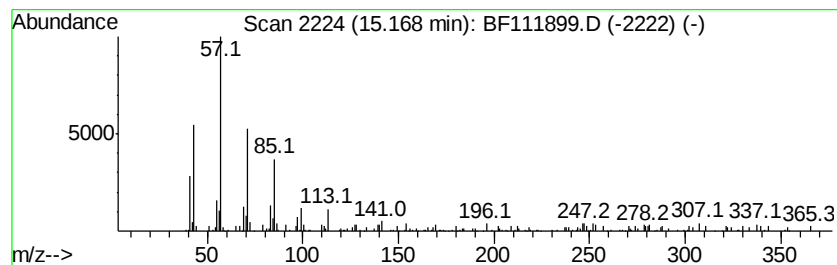
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
15.17	2.64 ng	84190	Perylene-d12	15.54

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptadecane	240	C17H36	000629-78-7	92
2		Hexadecane	226	C16H34	000544-76-3	83
3		Tetracosane	338	C24H50	000646-31-1	83
4		Pentadecane	212	C15H32	000629-62-9	64
5		Octacosane	394	C28H58	000630-02-4	58



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF010719\
Data File : BF111899.D
Acq On : 8 Jan 2019 1:36
Operator : JU/SJ
Sample : K1044-02 5X
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CPSB-08(20-25)

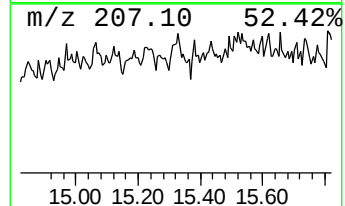
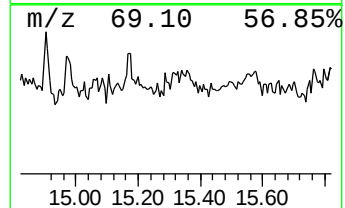
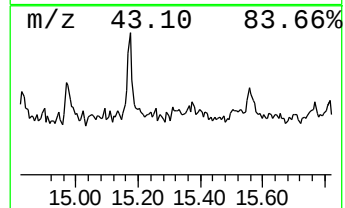
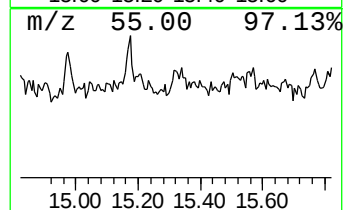
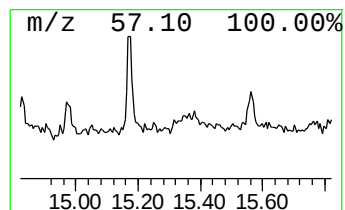
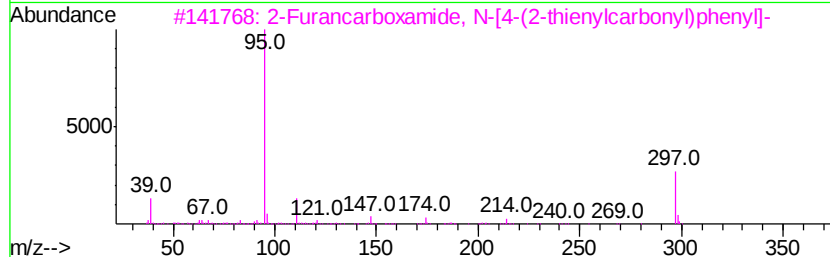
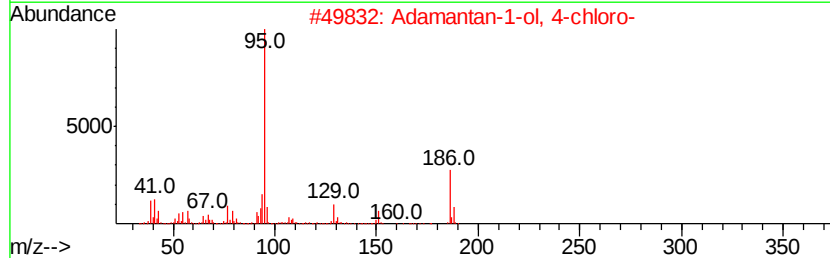
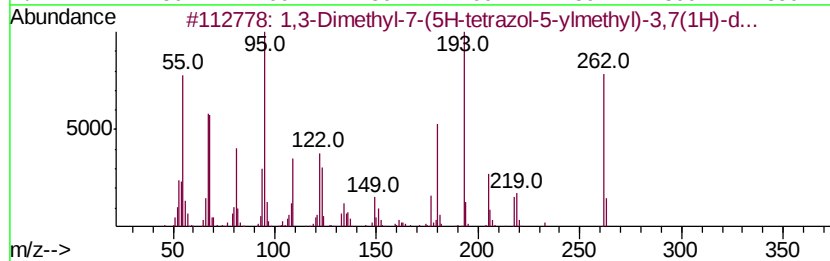
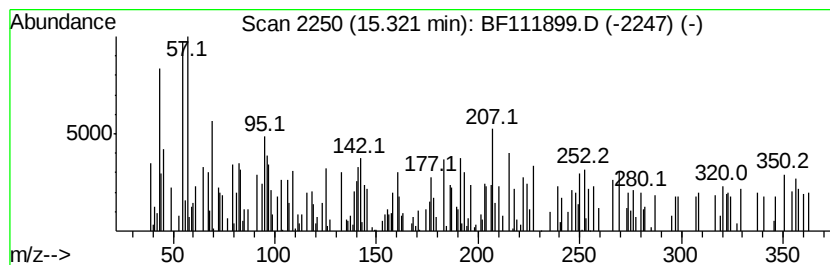
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 unknown15.32 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.32	2.12 ng	67624	Perylene-d12	15.54

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,3-Dimethyl-7-(5H-tetrazol-5-yl...	262	C9H10N8O2	1000297-46-0	30
2			Adamantan-1-ol, 4-chloro-	186	C10H15ClO	061357-37-7	25
3			2-Furancarboxamide, N-[4-(2-thie...	297	C16H11N03S	1000351-00-8	12
4			2H-Pyrrrol-2-one, 4-acetyl-1,5-di...	317	C15H15N3O3S	1000350-21-6	11
5			Allopregnan-9.alpha.-ol-3,20-dione	332	C21H32O3	1000251-12-1	11



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF010719\
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Acq On : 8 Jan 2019 1:36
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Sample : K1044-02 5X
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CPSB-08(20-25)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF010719.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
unknown6.66	6.66	13.9	ng	459289	1	6.89	662269	20.0
Tridecane, 3-methyl-	10.79	2.5	ng	88071	4	11.42	705142	20.0
Octadecanal	13.69	4.1	ng	149691	5	14.06	733323	20.0
1-Dodecanol, 2-he...	13.90	3.9	ng	141760	5	14.06	733323	20.0
Heneicosane	14.52	2.7	ng	97373	5	14.06	733323	20.0
Heptadecane	15.17	2.6	ng	84190	6	15.54	637150	20.0
unknown15.32	15.32	2.1	ng	67624	6	15.54	637150	20.0