

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF071818\
 Data File : BF107486.D
 Acq On : 18 Jul 2018 19:07
 Operator : JU/SJ
 Sample : J4016-23
 Misc :
 ALS Vial : 24 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB5-L-12-7

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-BF071618.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	5.231	487	492	501	rVB	345878	460466	13.13%	1.374%
2	5.619	551	558	561	rBV	3127357	3236606	92.28%	9.659%
3	6.613	721	727	730	rBV	3265427	3408262	97.17%	10.172%
4	6.754	746	751	755	rBV	3460290	3500900	99.81%	10.448%
5	6.984	786	790	794	rBV	1249958	993529	28.33%	2.965%
6	7.142	812	817	820	rBV	2852291	2518537	71.80%	7.516%
7	7.548	880	886	889	rBV	2367076	2227853	63.52%	6.649%
8	8.266	1004	1008	1014	rVB	1345173	1199646	34.20%	3.580%
9	9.342	1185	1191	1194	rBV	3894978	3507480	100.00%	10.468%
10	9.730	1253	1257	1262	rBV	635834	521578	14.87%	1.557%
11	9.942	1288	1293	1296	rVB2	38614	40618	1.16%	0.121%
12	10.030	1300	1308	1312	rBV	1424080	1318552	37.59%	3.935%
13	10.442	1376	1378	1380	rVB2	81224	57649	1.64%	0.172%
14	10.819	1437	1442	1446	rBV	2321249	2123018	60.53%	6.336%
15	10.913	1455	1458	1465	rVB3	67644	93580	2.67%	0.279%
16	11.366	1531	1535	1538	rBV3	55934	58307	1.66%	0.174%
17	11.519	1558	1561	1564	rBV	1311587	1223073	34.87%	3.650%
18	11.542	1564	1565	1570	rVV	219354	150414	4.29%	0.449%
19	11.595	1570	1574	1578	rVB2	40182	48771	1.39%	0.146%
20	12.024	1643	1647	1649	rBV4	43272	45603	1.30%	0.136%
21	12.142	1662	1667	1668	rBV3	36711	55113	1.57%	0.164%
22	12.736	1765	1768	1772	rBV	249813	199314	5.68%	0.595%
23	12.948	1801	1804	1805	rBV3	46930	44096	1.26%	0.132%
24	12.966	1805	1807	1814	rVB2	218038	299451	8.54%	0.894%
25	13.107	1826	1831	1834	rBV	2939770	2708257	77.21%	8.083%
26	13.401	1876	1881	1884	rBV7	21693	41089	1.17%	0.123%
27	13.471	1887	1893	1896	rBV	249507	258419	7.37%	0.771%
28	13.666	1922	1926	1929	rBV6	38114	46828	1.34%	0.140%
29	13.895	1962	1965	1972	rBV4	170045	186943	5.33%	0.558%
30	13.983	1977	1980	1984	rVB4	342670	315821	9.00%	0.943%
31	14.166	2007	2011	2014	rBV	1045576	1075362	30.66%	3.209%
32	14.195	2014	2016	2023	rVB	101318	128271	3.66%	0.383%
33	14.524	2069	2072	2074	rBV4	36657	47782	1.36%	0.143%
34	14.618	2085	2088	2091	rBV4	79293	82258	2.35%	0.245%

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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	14.942	2138	2143	2145	rBV6	75044	103843	2.96%	0.310%
36	15.248	2192	2195	2197	rBV2	57611	64174	1.83%	0.192%
37	15.295	2201	2203	2209	rVB7	71756	96606	2.75%	0.288%
38	15.707	2268	2273	2279	rBV2	674820	899553	25.65%	2.685%
39	16.177	2349	2353	2358	rBV8	64689	119956	3.42%	0.358%

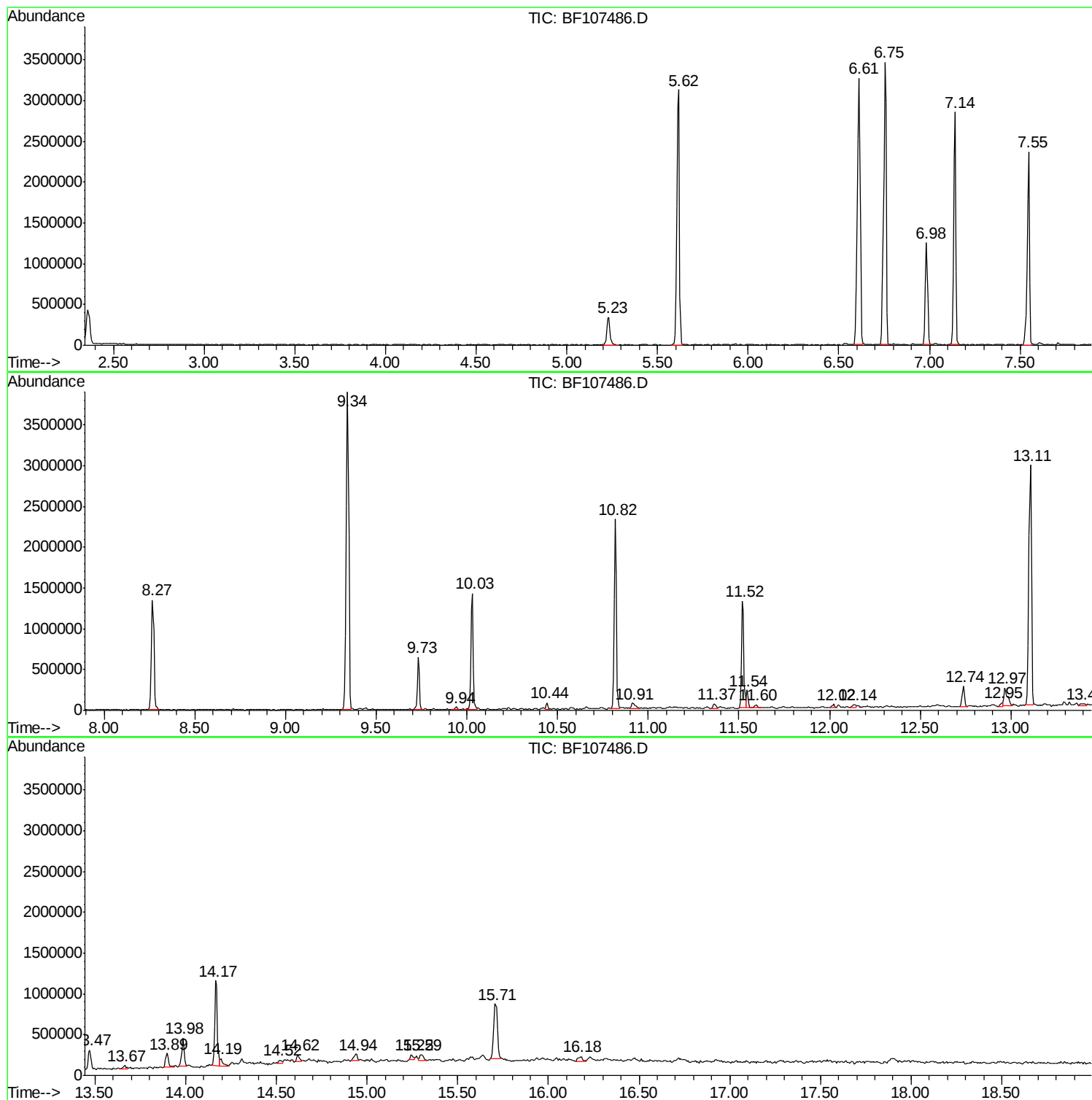
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF071618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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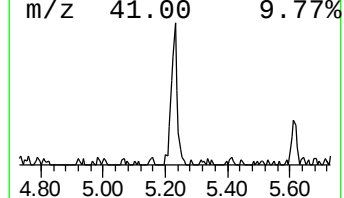
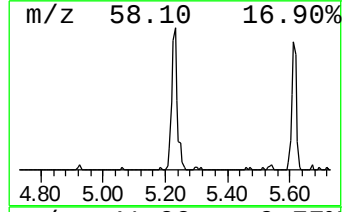
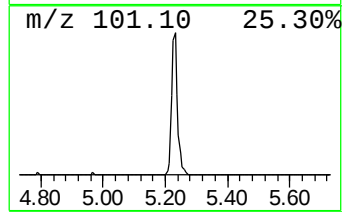
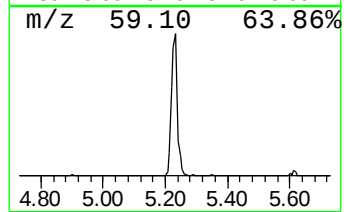
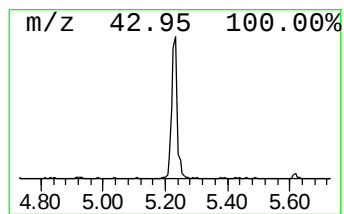
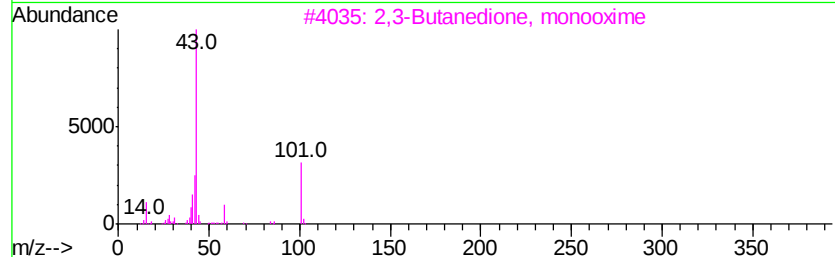
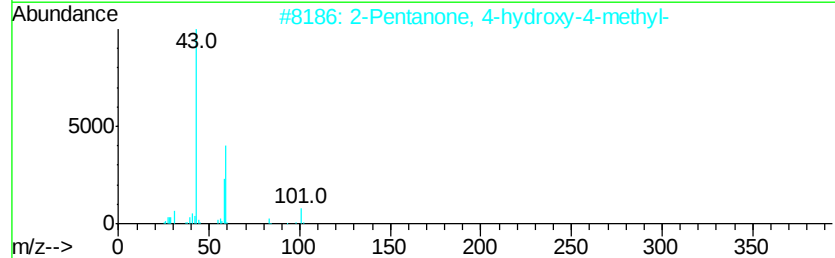
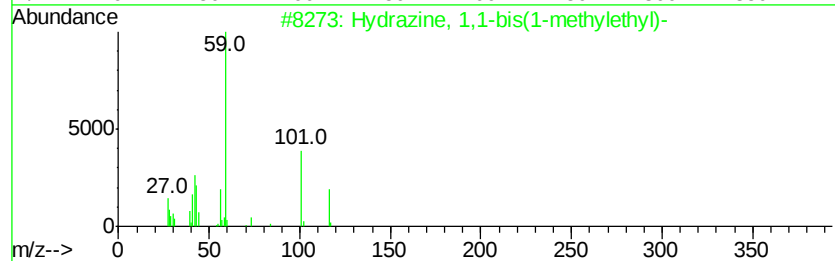
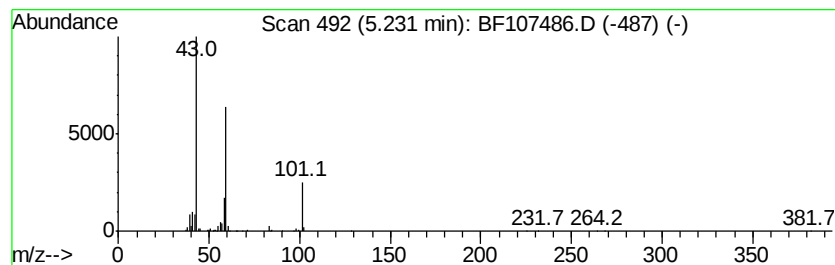
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF071618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown5.23 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.23	9.27 ng	460466	1,4-Dichlorobenzene-d4	6.98

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hydrazine, 1,1-bis(1-methylethyl)-	116	C6H16N2	000921-14-2	40
2			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	33
3			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	32
4			1,2-Butanediol	90	C4H10O2	000584-03-2	25
5			1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	23



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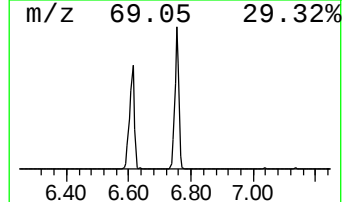
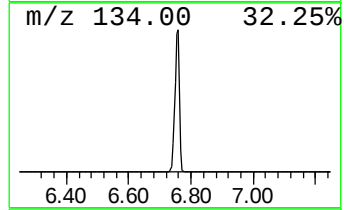
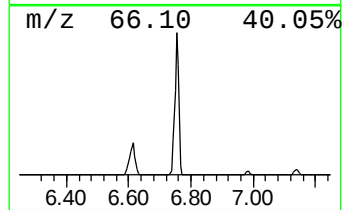
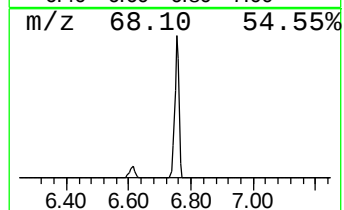
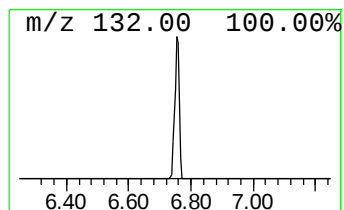
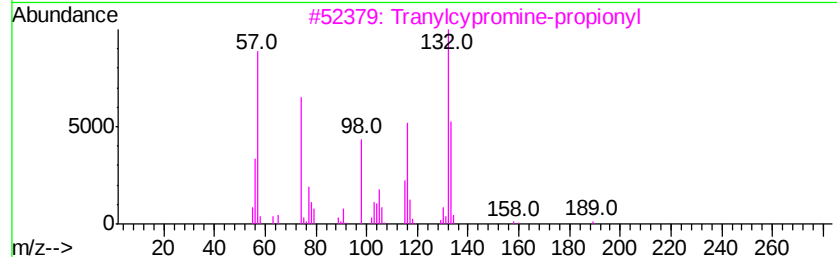
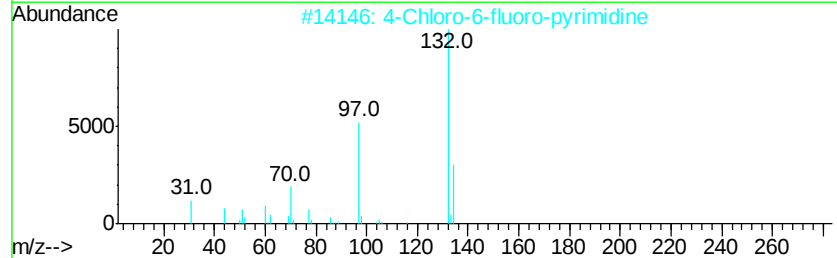
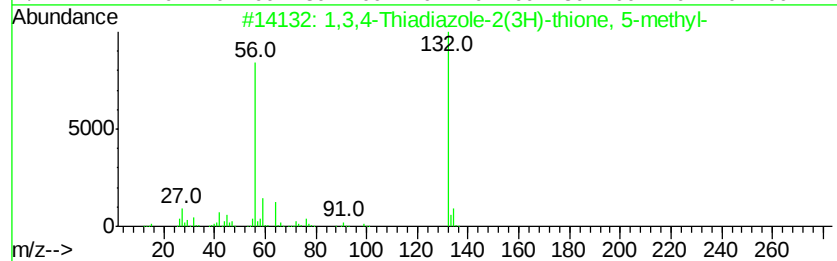
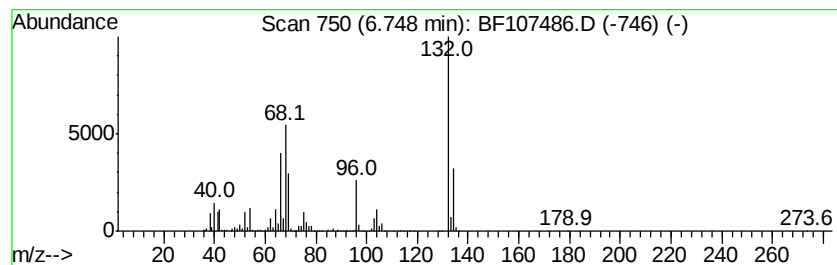
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 2 unknown6.75 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.75	70.47 ng	3500900	1,4-Dichlorobenzene-d4	6.98

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	14
2		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	14
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	10
4		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	10
5		1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	10



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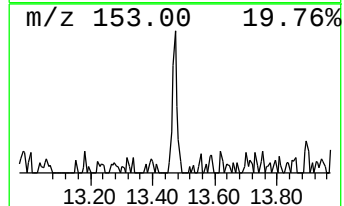
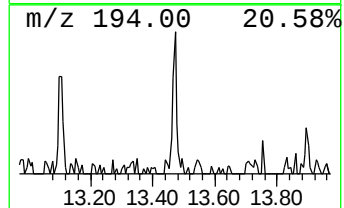
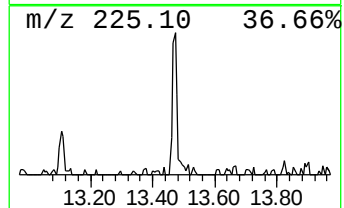
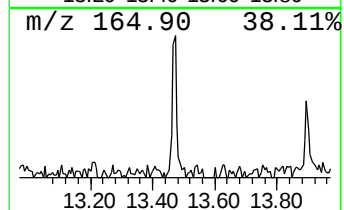
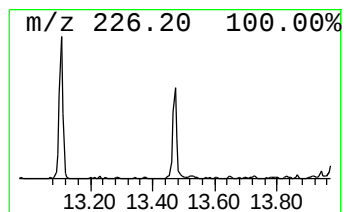
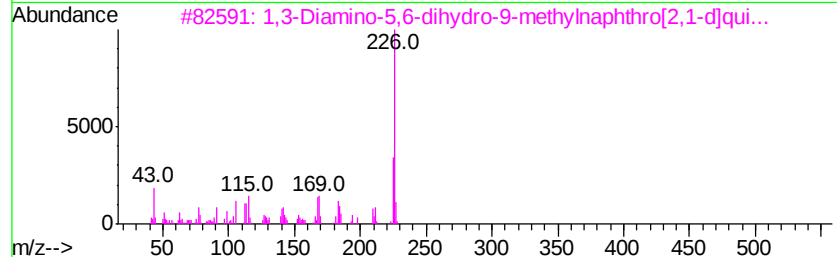
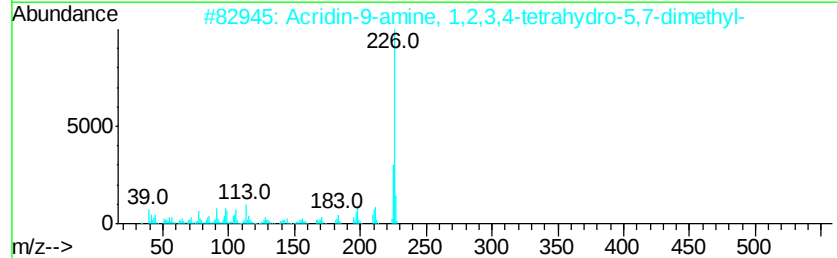
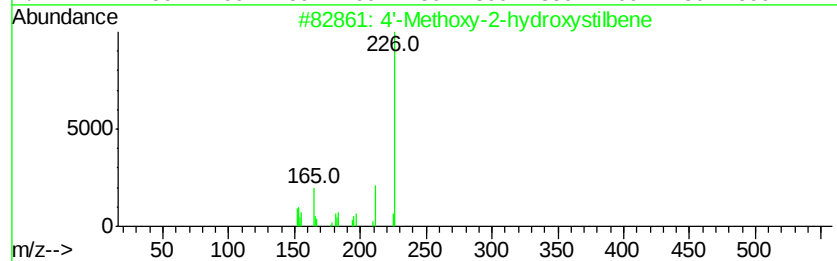
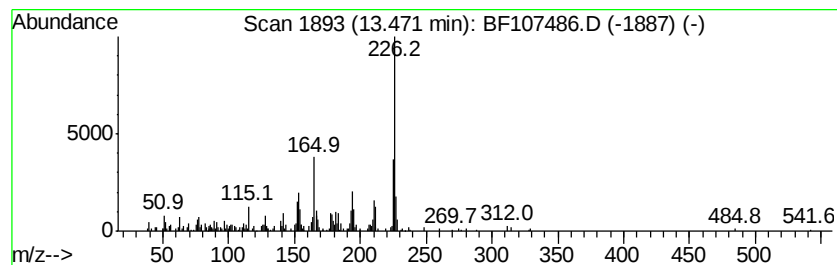
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF071618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 4'-Methoxy-2-hydroxystilbene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.47	4.81 ng	258419	Chrysene-d12	14.17	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4'-Methoxy-2-hydroxystilbene	226	C15H14O2	1000147-93-1	70
2	Acridin-9-amine, 1,2,3,4-tetrahy...	226	C15H18N2	1000300-57-6	55
3	1,3-Diamino-5,6-dihydro-9-methyl...	226	C13H14N4	037436-39-8	49
4	1,3-Diamino-5,6-dihydro-7-methyl...	226	C13H14N4	037436-37-6	49
5	9H-Pyrido[3,4-b]indole, 7-methox...	226	C14H14N2O	143502-37-8	49



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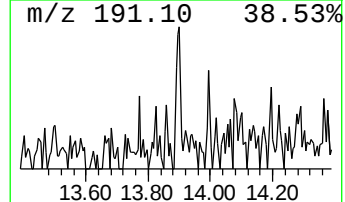
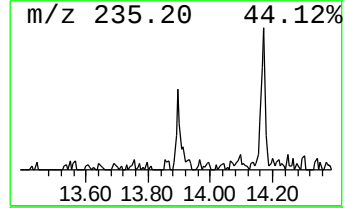
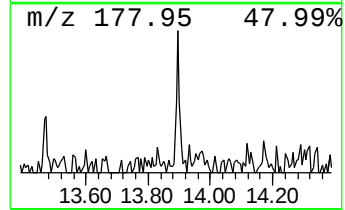
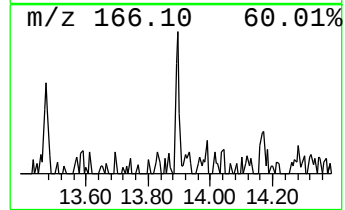
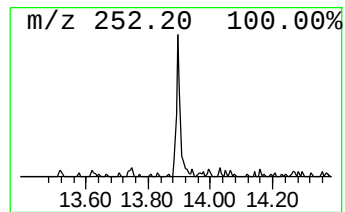
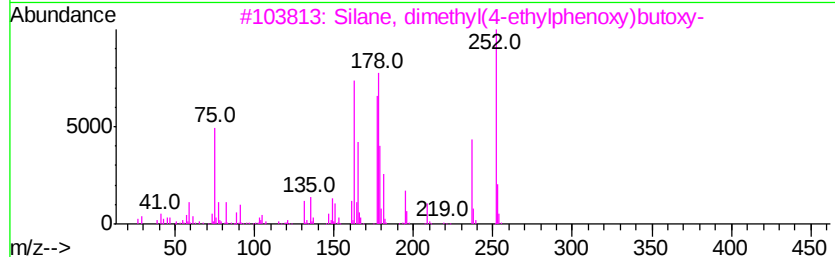
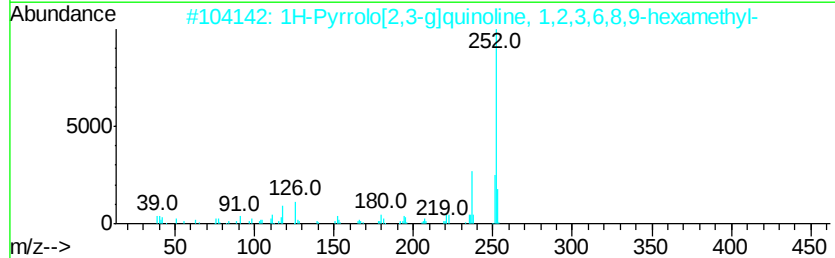
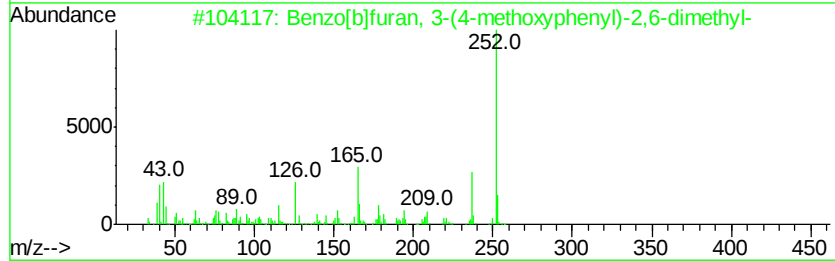
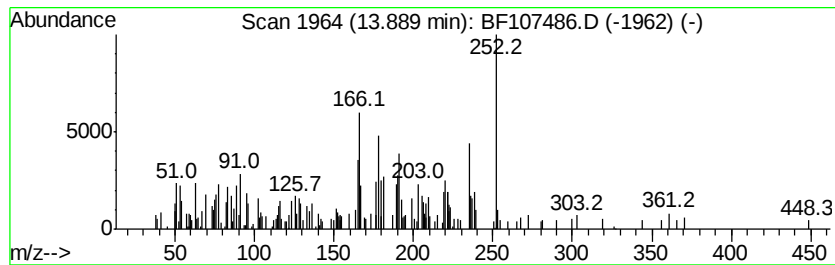
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 unknown13.89 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.89	3.48 ng	186943	Chrysene-d12	14.17

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzo[b]furan, 3-(4-methoxyphenyl)-2,6-dimethyl-	252	C17H16O2	074228-98-1	49
2		1H-Pyrrolo[2,3-g]quinoline, 1,2,3,6,8,9-hexamethyl-	252	C17H20N2	1000338-03-4	38
3		Silane, dimethyl(4-ethylphenoxy)butoxy-	252	C14H24O2Si	1000347-42-4	38
4		3H-Pyrrolo[3,2-f]quinoline, 1,2,3,6,8,9-hexamethyl-	252	C17H20N2	1000302-73-4	38
5		3-Hydroxyphenylacetic acid, ethyl ester	252	C13H20O3Si	067903-48-4	35



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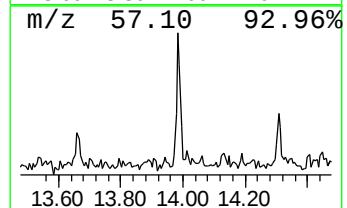
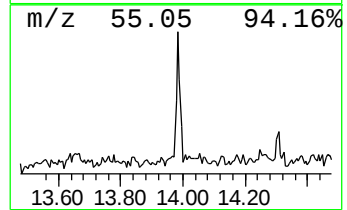
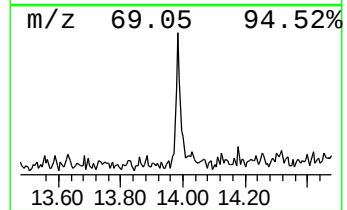
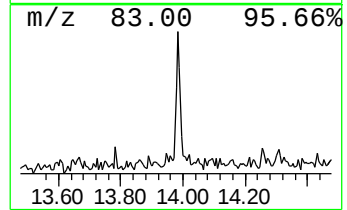
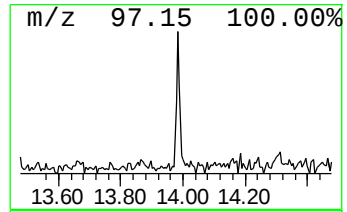
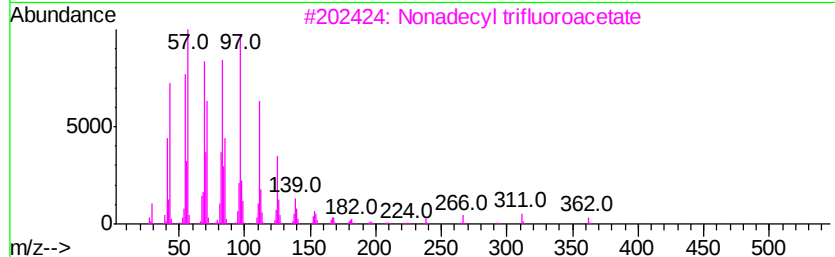
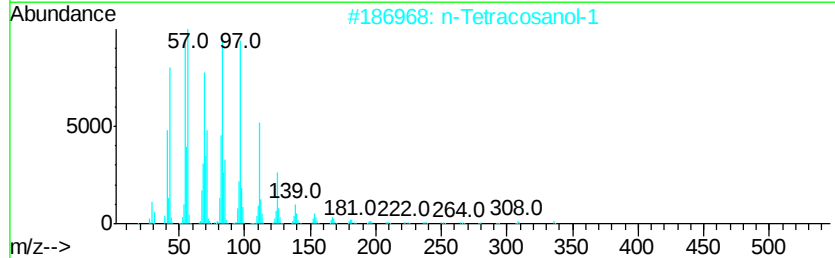
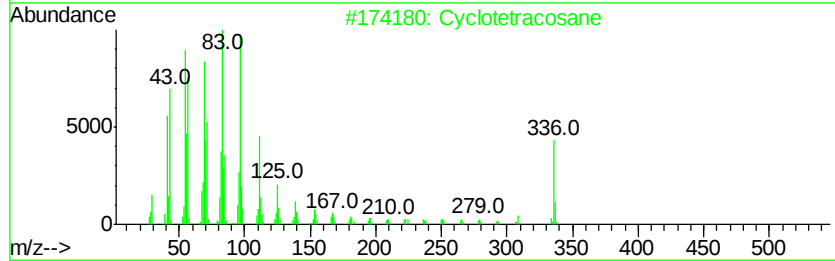
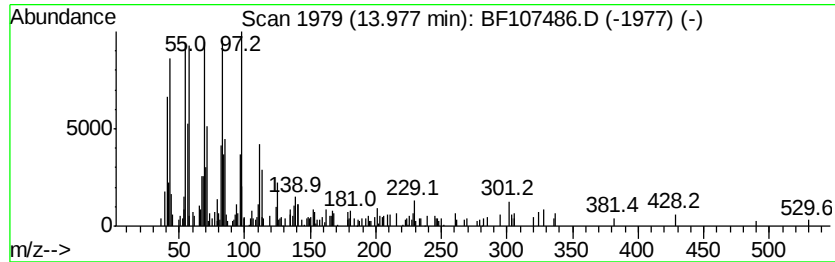
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Cyclotetracosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.98	5.87 ng	315821	Chrysene-d12	14.17

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cyclotetracosane	336	C24H48	000297-03-0	97
2		n-Tetracosanol-1	354	C24H50O	000506-51-4	95
3		Nonadecyl trifluoroacetate	380	C21H39F3O2	1000351-76-3	91
4		17-Pentatriacontene	491	C35H70	006971-40-0	91
5		1-Heptacosanol	396	C27H56O	002004-39-9	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF071818\
Data File : BF107486.D
Acq On : 18 Jul 2018 19:07
Operator : JU/SJ
Sample : J4016-23
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB5-L-12-7

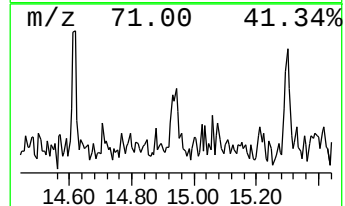
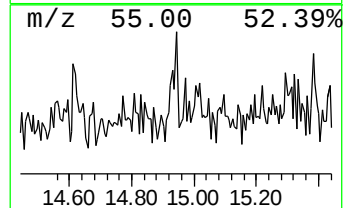
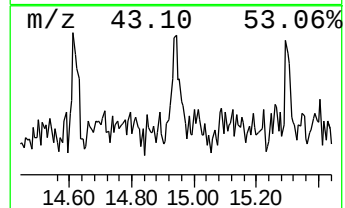
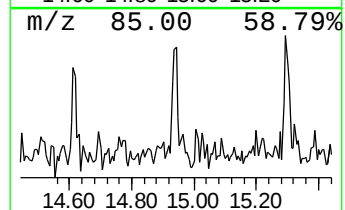
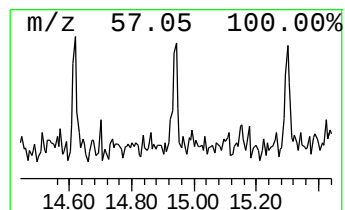
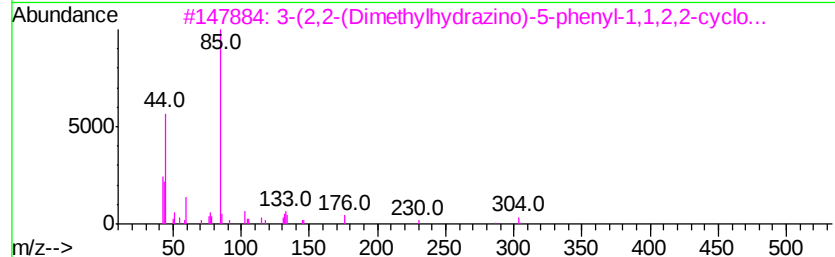
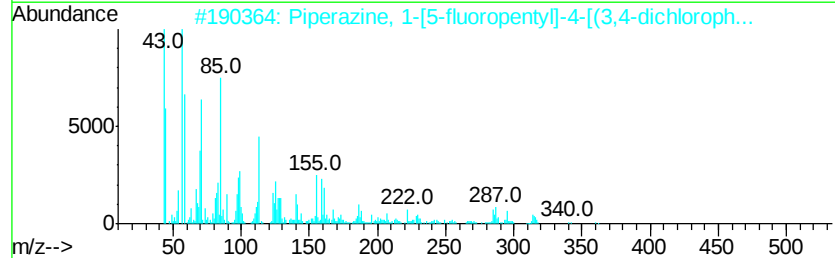
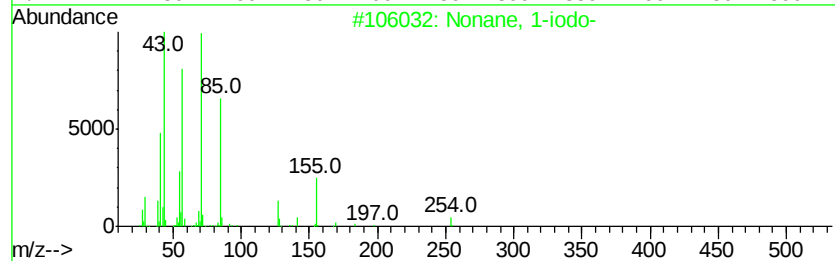
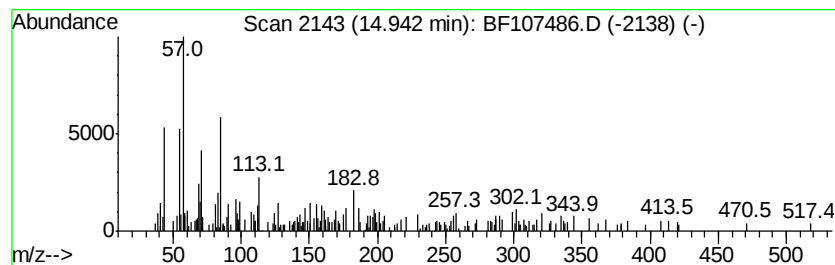
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown14.94 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.94	2.31 ng	103843	Perylene-d12	15.71

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Nonane, 1-iodo-	254	C9H19I	004282-42-2	38
2		Piperazine, 1-[5-fluoropentyl]-4...	360	C17H23Cl2FN2O	141044-94-2	38
3		3-(2,2-(Dimethylhydrazino)-5-phe...	304	C17H16N6	1000326-95-3	38
4		Octadecane	254	C18H38	000593-45-3	38
5		Pentane, 1-bromo-3-methyl-	164	C6H13Br	051116-73-5	38



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF071818\
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Operator : JU/SJ
Sample : J4016-23
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB5-L-12-7

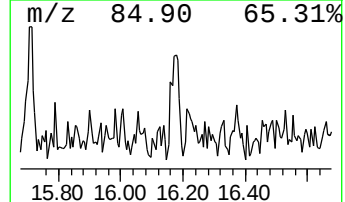
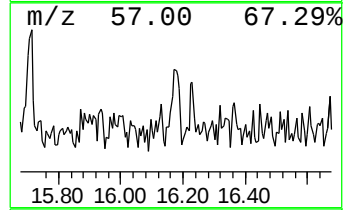
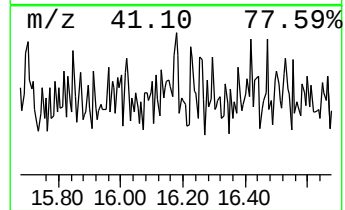
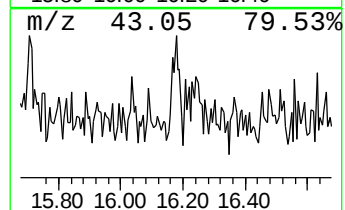
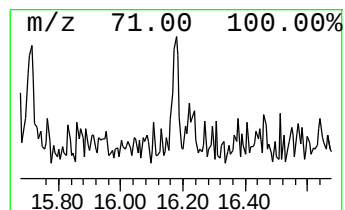
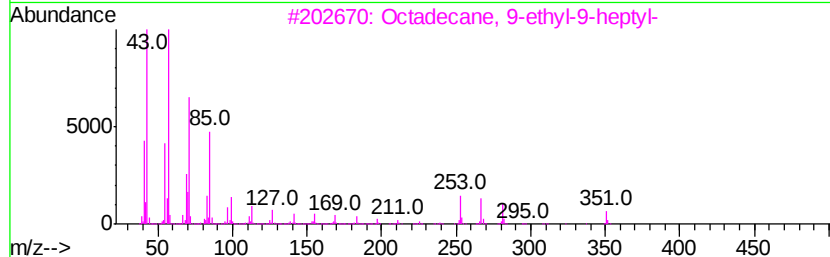
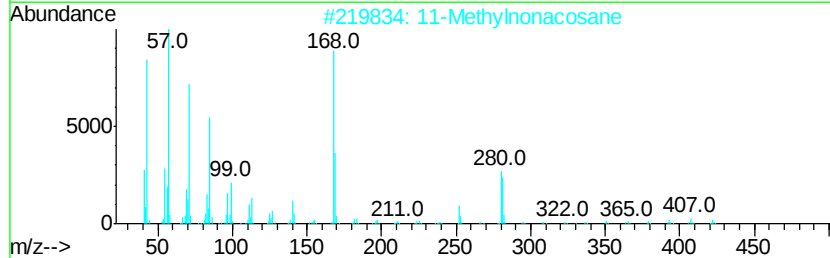
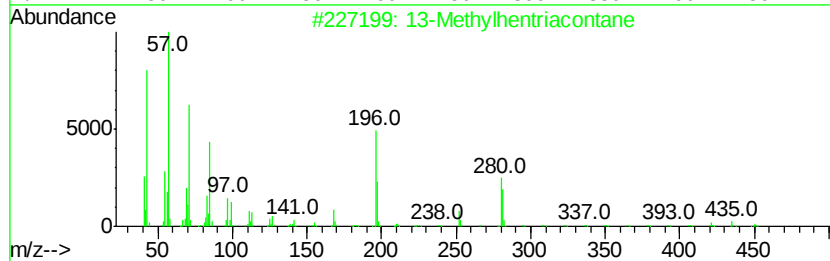
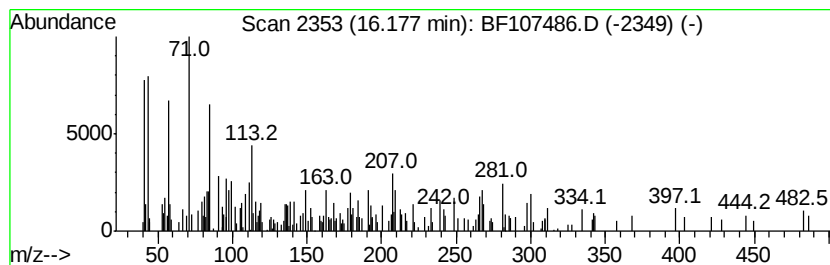
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown16.18 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.18	2.67 ng	119956	Perylene-d12	15.71

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	13-Methylhentriacontane	451	C32H66	1000131-19-4	43
2		11-Methylnonacosane	422	C30H62	007371-99-5	40
3		Octadecane, 9-ethyl-9-heptyl-	380	C27H56	055282-27-4	38
4		Hexadecane, 8-hexyl-8-pentyl-	380	C27H56	055282-29-6	37
5		Octadecane, 3-ethyl-5-(2-ethylbu...	366	C26H54	055282-12-7	33



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF071818\
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Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB5-L-12-7

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF071618.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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unknown6.75	6.75	70.5	ng	3500900	1	6.98	993529	20.0
4'-Methoxy-2-hydr...	13.47	4.8	ng	258419	5	14.17	1075360	20.0
unknown13.89	13.89	3.5	ng	186943	5	14.17	1075360	20.0
Cyclotetracosane	13.98	5.9	ng	315821	5	14.17	1075360	20.0
unknown14.94	14.94	2.3	ng	103843	6	15.71	899553	20.0
unknown16.18	16.18	2.7	ng	119956	6	15.71	899553	20.0