

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF062718\
 Data File : BF106878.D
 Acq On : 27 Jun 2018 18:01
 Operator : JU/SJ
 Sample : J3570-06
 Misc :
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 20180376-COMPOSITE-CS-1B-ELU

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-BF061918.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	5.190	481	485	492	rBB	26909	30687	2.03%	0.278%
2	5.589	550	553	557	rBV	700868	642559	42.47%	5.822%
3	6.589	719	723	734	rVB	514972	487577	32.23%	4.418%
4	6.731	742	747	750	rBV	1121111	1054736	69.71%	9.557%
5	6.954	781	785	788	rBV	329603	275421	18.20%	2.496%
6	7.001	790	793	801	rBB	95429	74540	4.93%	0.675%
7	7.113	807	812	815	rBV	1016689	984600	65.08%	8.922%
8	7.354	849	853	857	rBV	18444	15568	1.03%	0.141%
9	7.519	873	881	884	rBV	750712	825269	54.55%	7.478%
10	7.619	890	898	902	rVB3	10520	18710	1.24%	0.170%
11	8.236	999	1003	1015	rBV	398942	356753	23.58%	3.233%
12	9.313	1179	1186	1189	rBV	1537607	1512991	100.00%	13.710%
13	9.701	1248	1252	1258	rVB	186568	150315	9.93%	1.362%
14	9.901	1282	1286	1291	rBV2	25403	24235	1.60%	0.220%
15	9.995	1298	1302	1306	rBV	489392	417871	27.62%	3.786%
16	10.401	1369	1371	1374	rVB	53825	40493	2.68%	0.367%
17	10.624	1403	1409	1411	rBV	13361	16982	1.12%	0.154%
18	10.654	1411	1414	1417	rBV	178287	128885	8.52%	1.168%
19	10.789	1433	1437	1441	rBV	963704	1027602	67.92%	9.311%
20	10.877	1449	1452	1462	rVB2	48749	57640	3.81%	0.522%
21	10.954	1462	1465	1467	rBV	17967	15927	1.05%	0.144%
22	10.983	1467	1470	1474	rVB3	16239	19536	1.29%	0.177%
23	11.024	1474	1477	1479	rBV	17920	15813	1.05%	0.143%
24	11.171	1499	1502	1504	rBV	20385	16360	1.08%	0.148%
25	11.324	1526	1528	1531	rBV	24111	18465	1.22%	0.167%
26	11.489	1552	1556	1559	rBV	484754	441702	29.19%	4.002%
27	11.636	1578	1581	1584	rBV	41744	35345	2.34%	0.320%
28	12.036	1646	1649	1654	rVB2	17170	16585	1.10%	0.150%
29	12.495	1724	1727	1732	rBV	19973	18612	1.23%	0.169%
30	13.077	1820	1826	1829	rBV	1379143	1500877	99.20%	13.600%
31	13.948	1971	1974	1978	rBV	36734	35370	2.34%	0.320%
32	14.136	2002	2006	2011	rBV	333012	322693	21.33%	2.924%
33	14.983	2146	2150	2155	rBV2	44326	53980	3.57%	0.489%
34	15.677	2262	2268	2275	rBV	269529	341887	22.60%	3.098%

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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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35	15.936	2306	2312	2325	rVB	10589	39478	2.61%	0.358%
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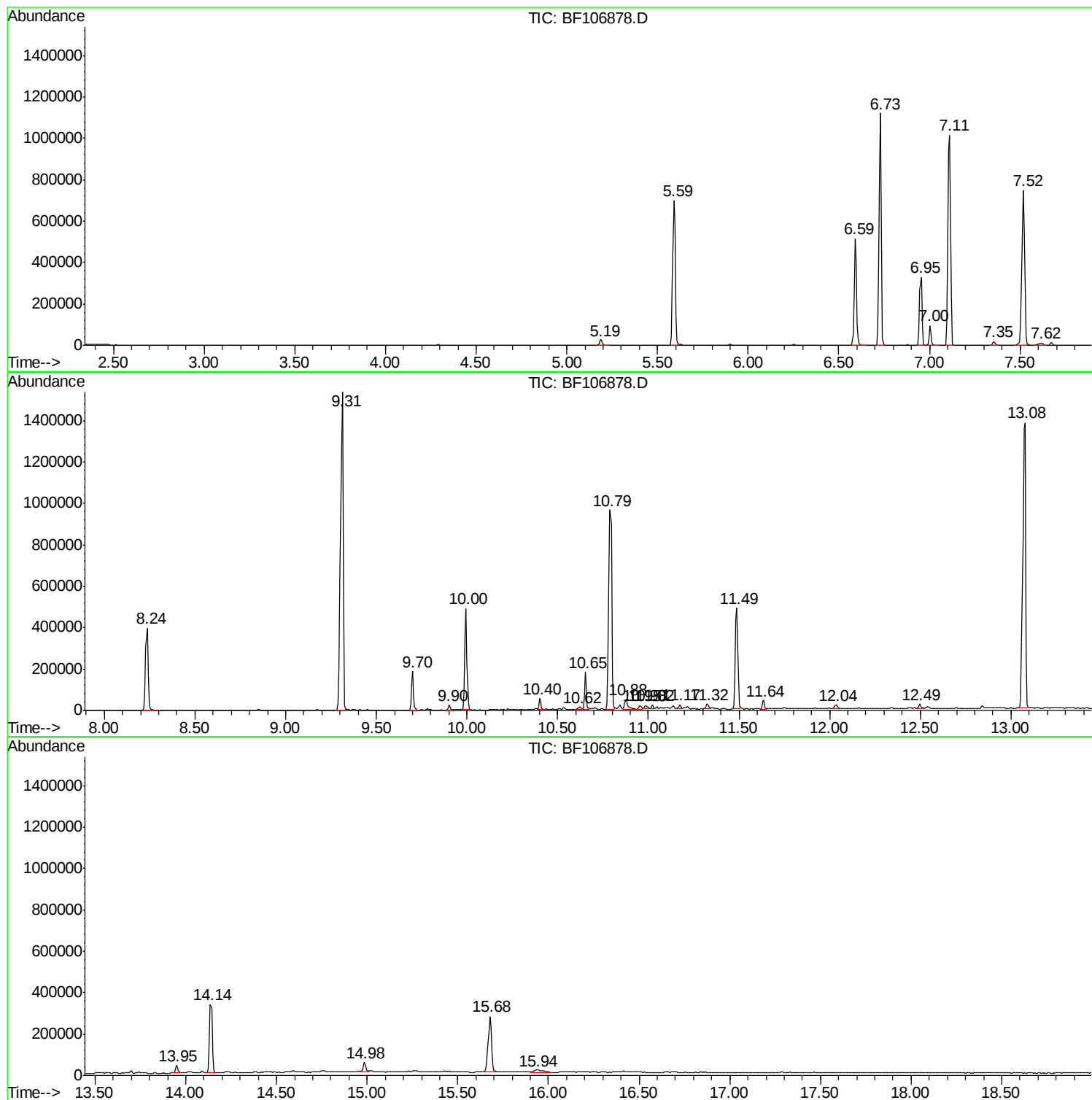
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF061918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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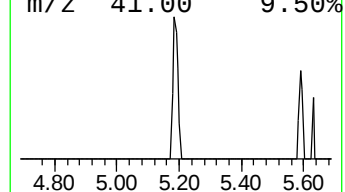
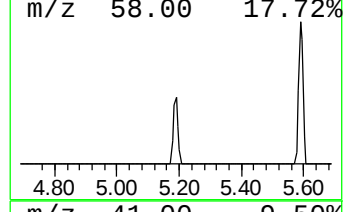
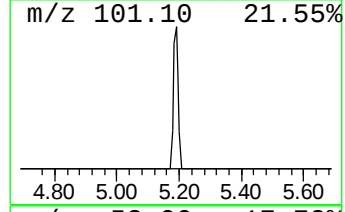
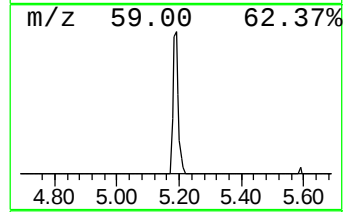
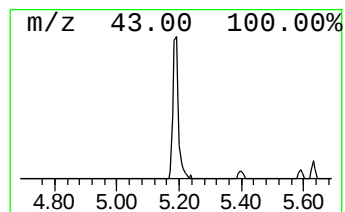
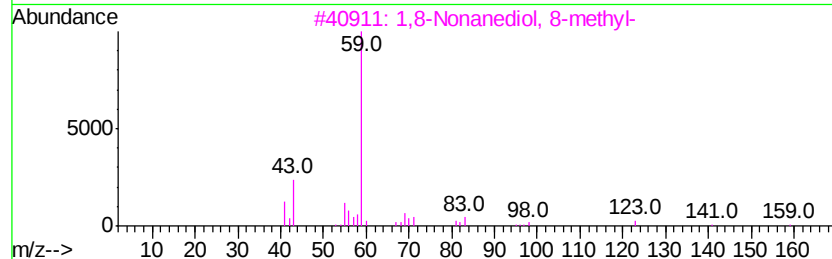
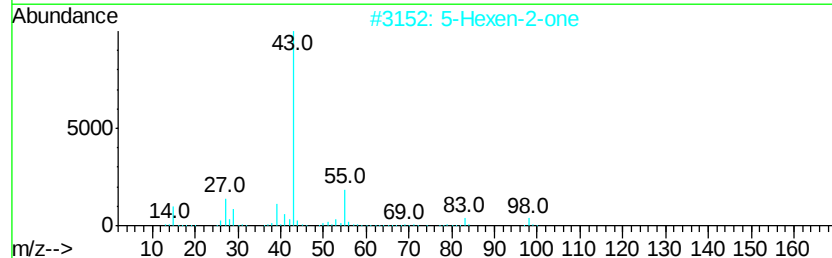
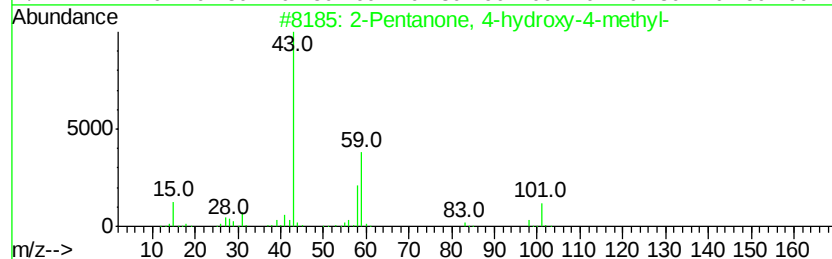
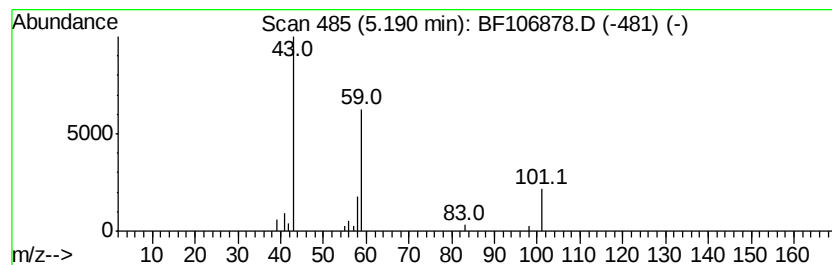
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.19	2.23 ng	30687	1,4-Dichlorobenzene-d4	6.95

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56		
2	5-Hexen-2-one	98	C6H10O	000109-49-9	9		
3	1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	9		
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9		
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	5		



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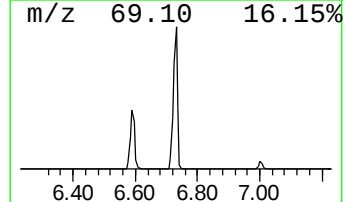
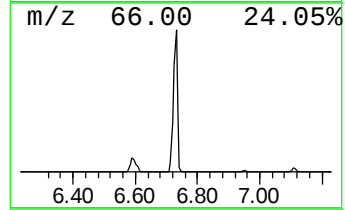
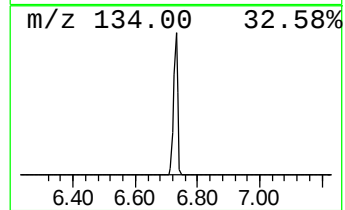
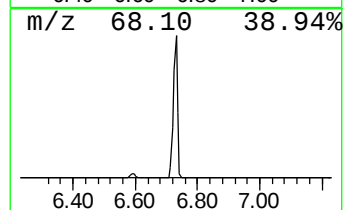
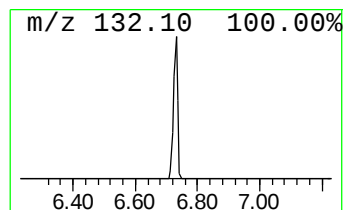
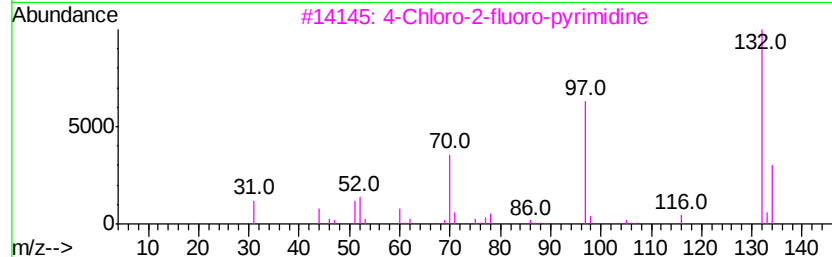
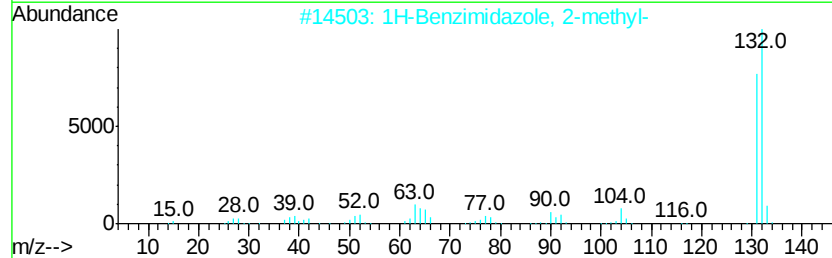
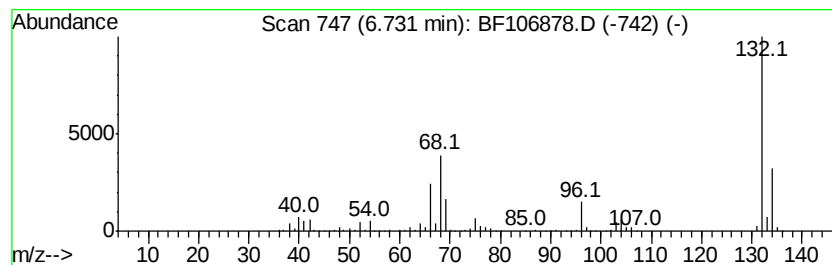
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.73 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.73	76.59 ng	1054740	1,4-Dichlorobenzene-d4	6.95

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	3	Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
2	1H-Benzimidazole, 2-methyl-		132	C8H8N2	000615-15-6	10
3	4-Chloro-2-fluoro-pyrimidine		132	C4H2ClFN2	051422-00-5	9
4	1-Methylpyrrolo[1,2-a]pyrazine		132	C8H8N2	064608-59-9	9
5	4-Methylpyrrolo[1,2-a]pyrazine		132	C8H8N2	064608-60-2	9



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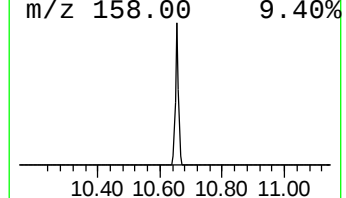
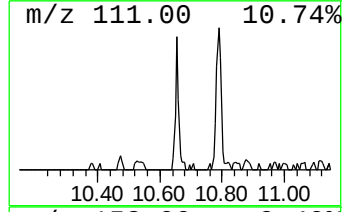
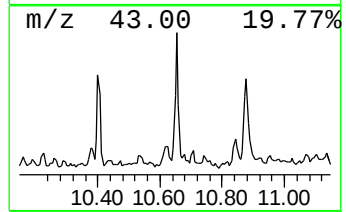
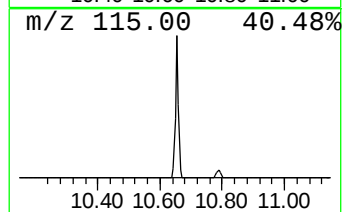
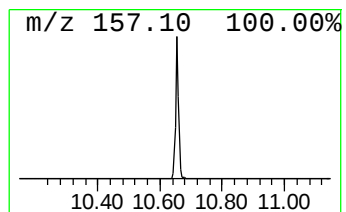
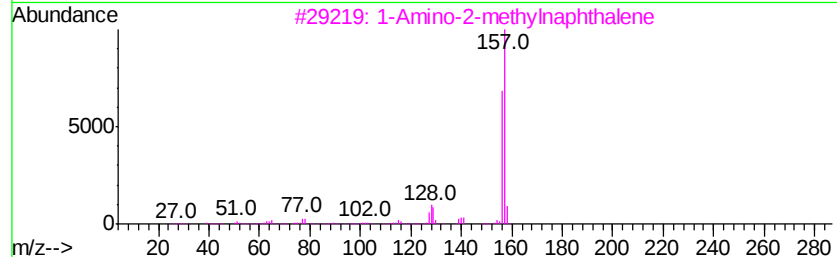
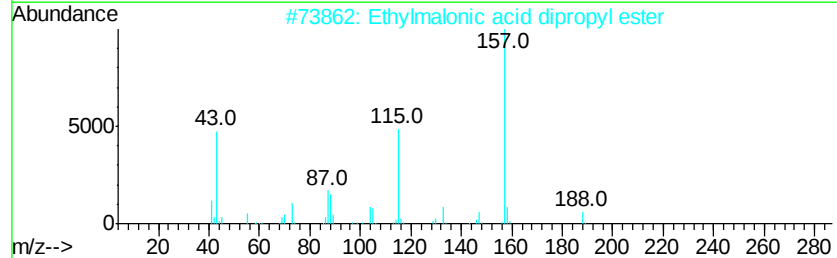
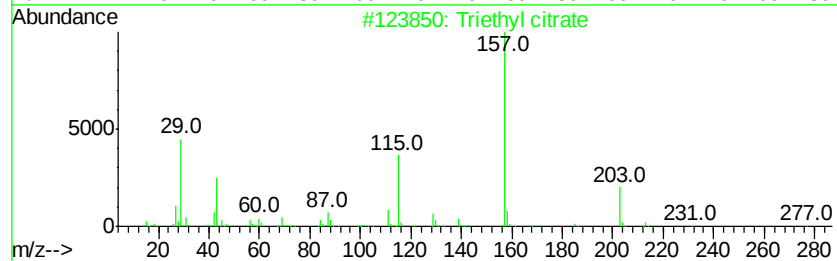
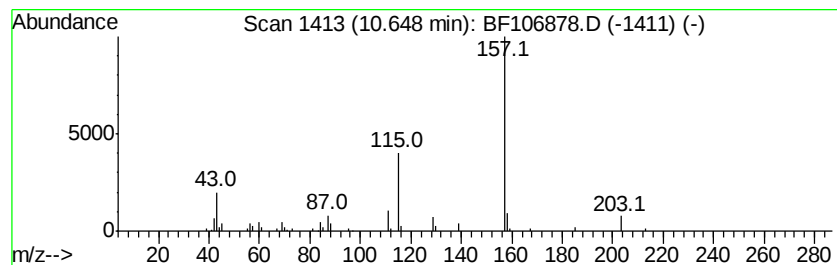
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Triethyl citrate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD		R.T.	
10.65	6.17 ng	128885	Acenaphthene-d10		10.00	
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Triethyl citrate	276	C12H20O7	000077-93-0	90
2		Ethylmalonic acid dipropyl ester	216	C11H20O4	001113-91-3	64
3		1-Amino-2-methylnaphthalene	157	C11H11N	002246-44-8	40
4		3-Chloro2-fluorobenzoic acid, 4-...	356	C20H30ClF02	1000338-64-4	38
5		Adipic acid, ethyl 4-methylpent-...	258	C14H26O4	1000353-49-9	36



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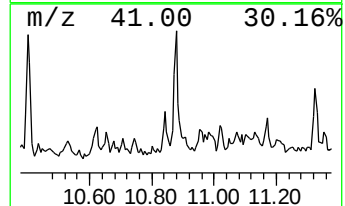
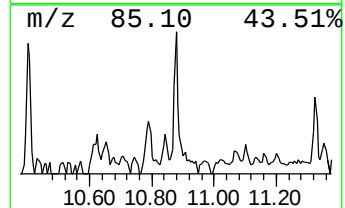
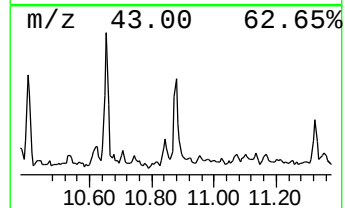
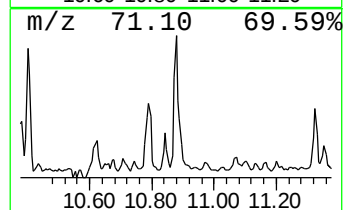
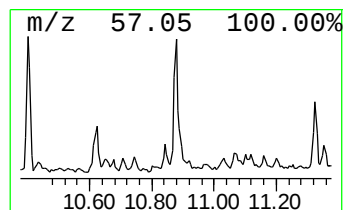
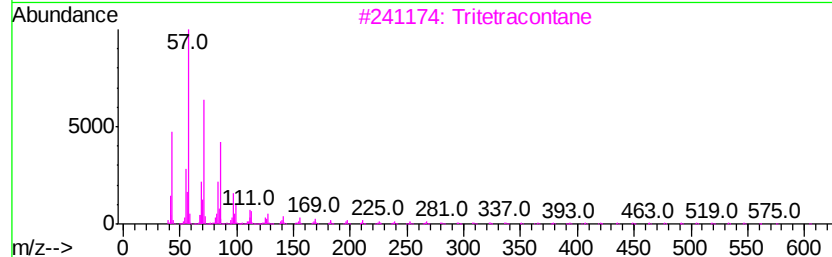
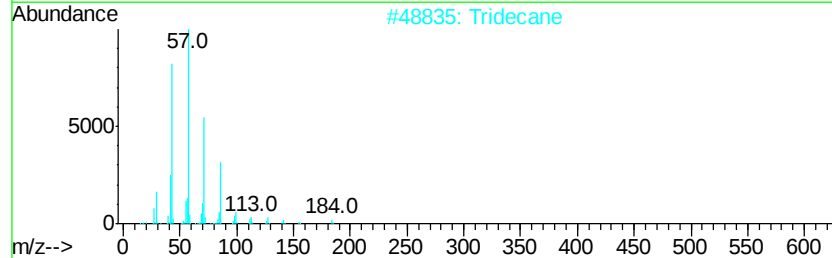
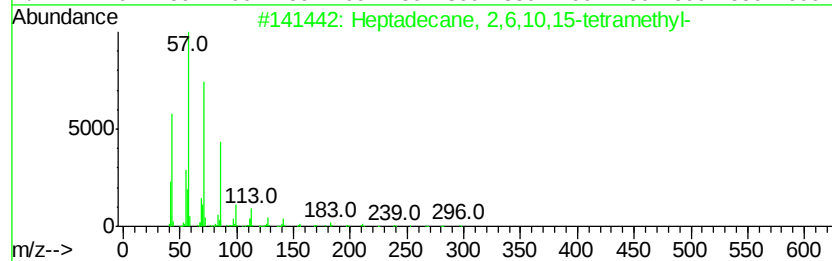
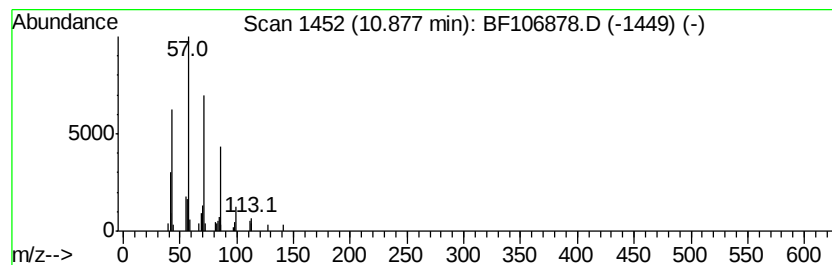
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Heptadecane, 2,6,10,15-tetr... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.88	2.61 ng	57640	Phenanthrene-d10	11.49

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	90
2		Tridecane	184	C13H28	000629-50-5	90
3		Tritetracontane	605	C43H88	007098-21-7	90
4		Tetradecane	198	C14H30	000629-59-4	90
5		Heptadecane	240	C17H36	000629-78-7	86



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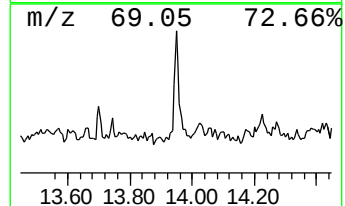
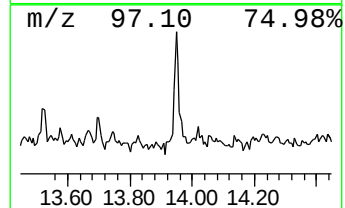
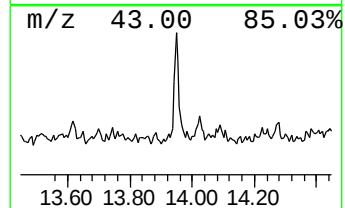
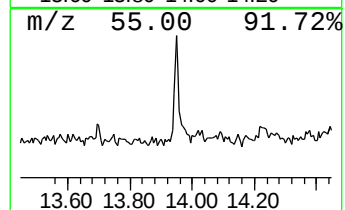
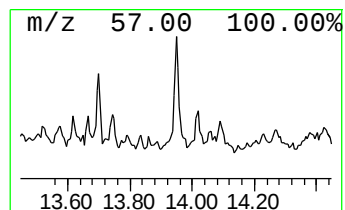
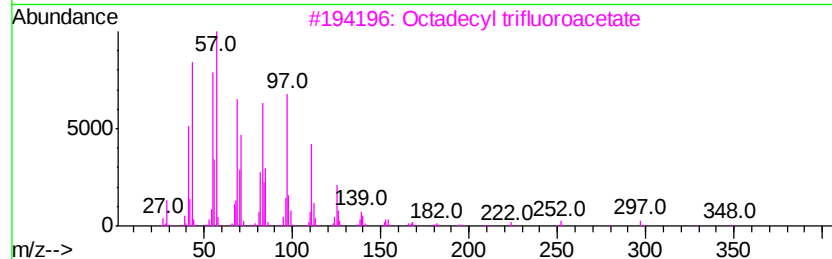
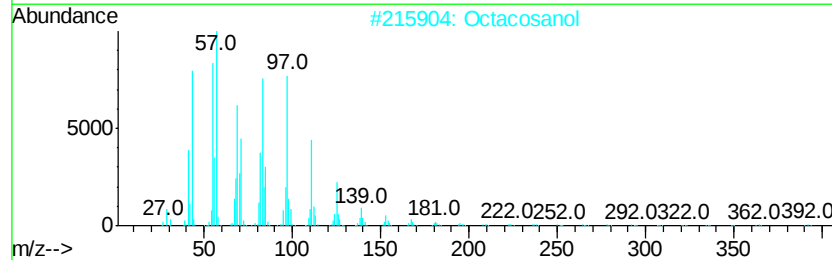
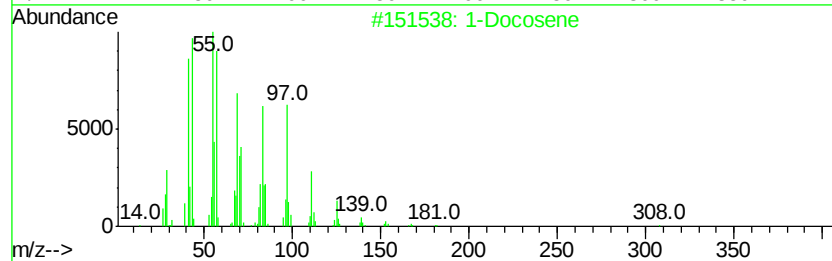
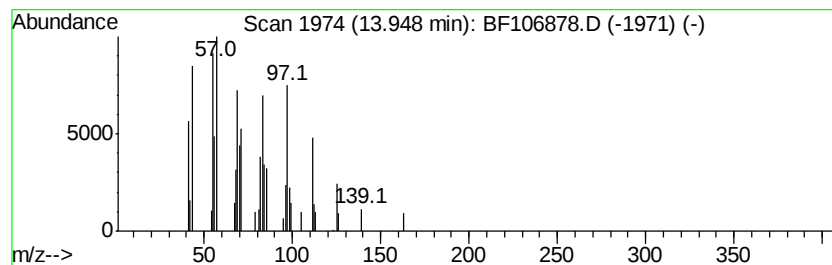
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Peak Number 6 1-Docosene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.95	2.19 ng	35370	Chrysene-d12	14.14

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Docosene	308	C22H44	001599-67-3	91
2		Octacosanol	410	C28H58O	000557-61-9	91
3		Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	91
4		Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	91
5		Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF062718\
Data File : BF106878.D
Acq On : 27 Jun 2018 18:01
Operator : JU/SJ
Sample : J3570-06
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
20180376-COMPOSITE-CS-1B-ELU

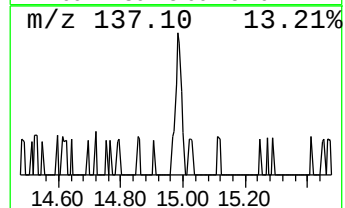
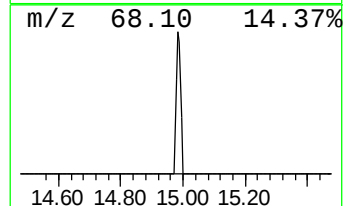
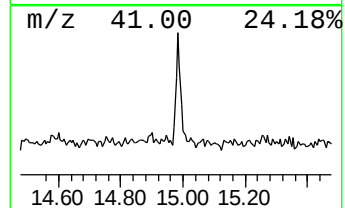
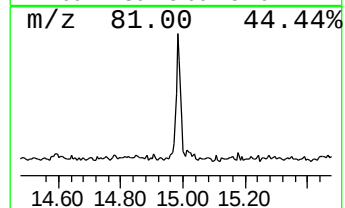
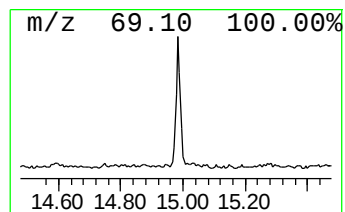
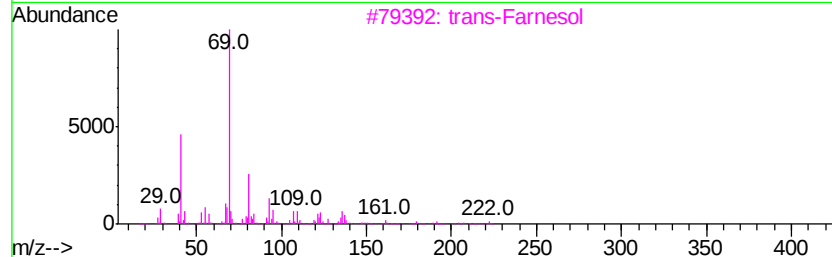
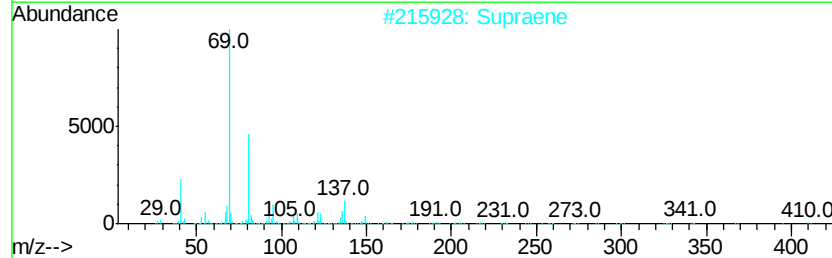
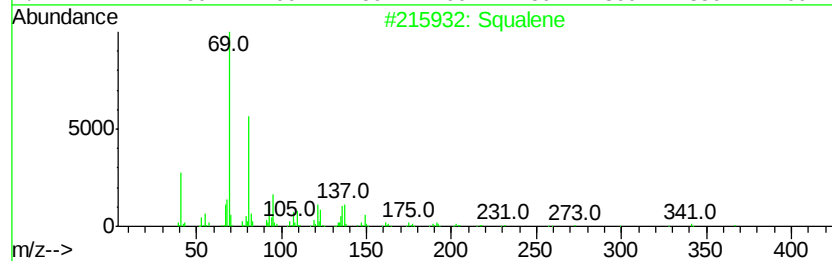
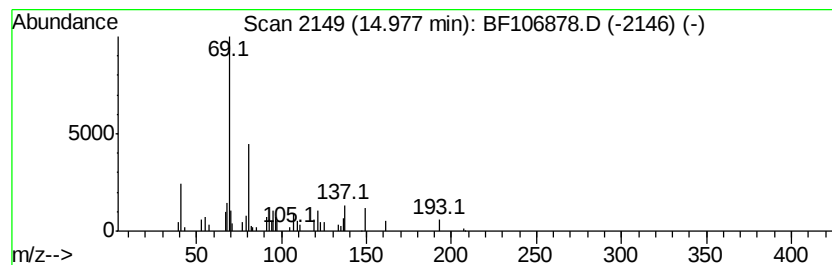
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Squalene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.98	3.16 ng	53980	Perylene-d12	15.68

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Squalene	410	C30H50	000111-02-4	86
2		Supraene	410	C30H50	007683-64-9	80
3		trans-Farnesol	222	C15H26O	000106-28-5	50
4		Succinic acid, di(3-methylbut-3-...	254	C14H22O4	1000353-45-6	47
5		1,5,9-Decatriene, 2,3,5,8-tetram...	192	C14H24	230646-72-7	45



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF062718\
Data File : BF106878.D
Acq On : 27 Jun 2018 18:01
Operator : JU/SJ
Sample : J3570-06
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
20180376-COMPOSITE-CS-1B-ELU

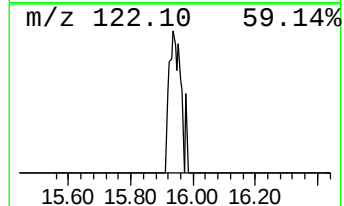
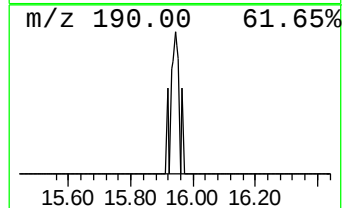
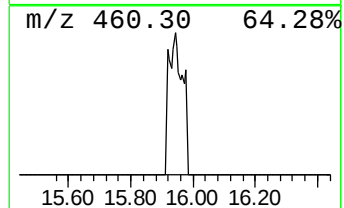
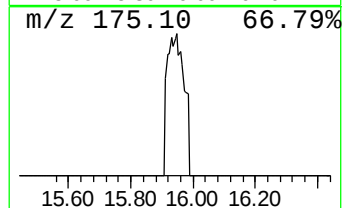
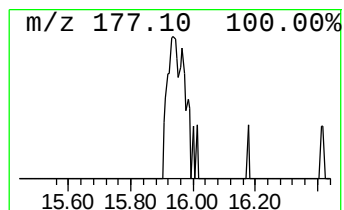
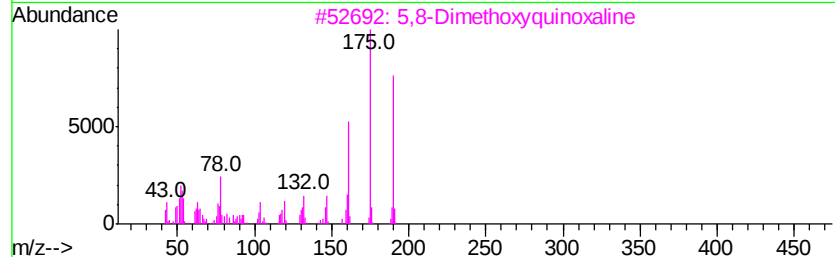
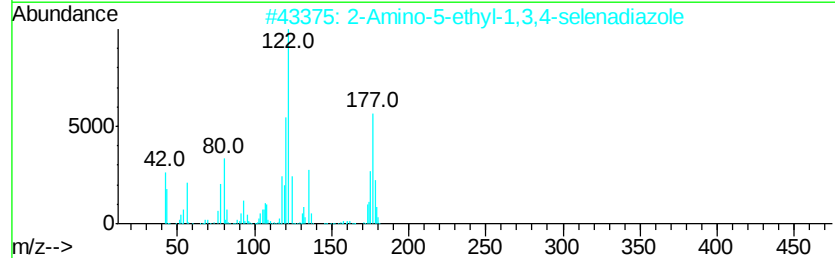
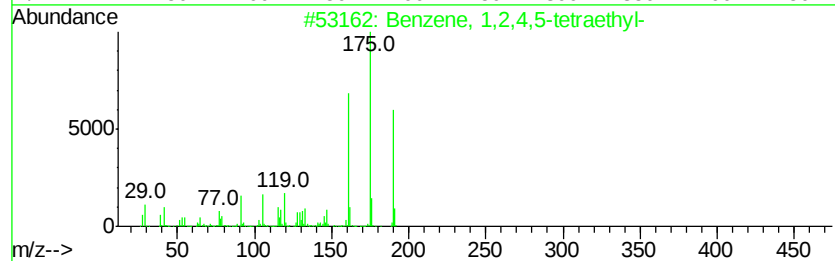
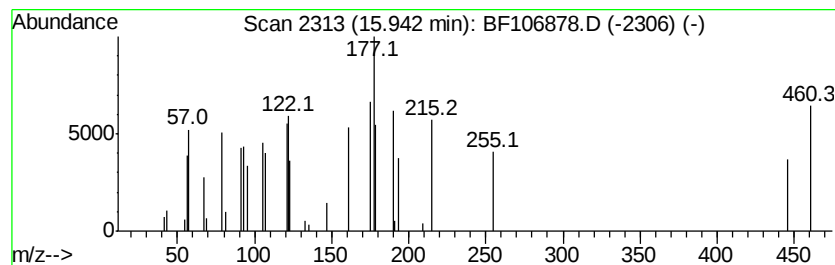
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Benzene, 1,2,4,5-tetraethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.94	2.31 ng	39478	Perylene-d12	15.68

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzene, 1,2,4,5-tetraethyl-	190	C14H22	000635-81-4	14
2		2-Amino-5-ethyl-1,3,4-selenadiazole	177	C4H7N3Se	034547-85-8	12
3		5,8-Dimethoxyxvinoxaline	190	C10H10N2O2	019506-19-5	9
4		Luminol	177	C8H7N3O2	000521-31-3	9
5		Ibuprofen methyl ester	220	C14H20O2	061566-34-5	9



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF062718\
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Acq On : 27 Jun 2018 18:01
Operator : JU/SJ
Sample : J3570-06
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
20180376-COMPOSITE-CS-1B-ELU

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061918.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...	5.19	2.2	ng	30687	1	6.95	275421	20.0
unknown6.73	6.73	76.6	ng	1054740	1	6.95	275421	20.0
Triethyl citrate	10.65	6.2	ng	128885	3	10.00	417871	20.0
Heptadecane, 2,6,...	10.88	2.6	ng	57640	4	11.49	441702	20.0
1-Docosene	13.95	2.2	ng	35370	5	14.14	322693	20.0
Squalene	14.98	3.2	ng	53980	6	15.68	341887	20.0
Benzene, 1,2,4,5-...	15.94	2.3	ng	39478	6	15.68	341887	20.0