

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF071618\
 Data File : BF107430.D
 Acq On : 17 Jul 2018 3:52
 Operator : JU/SJ
 Sample : J3980-03
 Misc :
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP-E-MH-S

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	2.449	18	19	25	rVB5	27348	33694	1.30%	0.134%
2	5.219	486	490	495	rBV	282024	313730	12.14%	1.249%
3	5.607	551	556	559	rBV	2676734	2482600	96.03%	9.886%
4	6.607	720	726	733	rVB	2559272	2583812	99.95%	10.289%
5	6.754	746	751	754	rBV	2730479	2585178	100.00%	10.294%
6	6.801	755	759	763	rVB	43299	36113	1.40%	0.144%
7	6.984	786	790	793	rBV	1088317	870516	33.67%	3.466%
8	7.031	793	798	802	rVB3	28437	30930	1.20%	0.123%
9	7.137	812	816	820	rVB	2227527	1957782	75.73%	7.796%
10	7.543	880	885	888	rBV	1805549	1554293	60.12%	6.189%
11	7.713	911	914	918	rVB	35924	28210	1.09%	0.112%
12	8.266	1004	1008	1011	rBV	1180371	961362	37.19%	3.828%
13	9.336	1186	1190	1194	rBV	2599458	2372749	91.78%	9.448%
14	9.442	1205	1208	1211	rVB2	29294	28911	1.12%	0.115%
15	9.731	1254	1257	1260	rBV	603524	457102	17.68%	1.820%
16	10.025	1303	1307	1311	rBV	1159435	970642	37.55%	3.865%
17	10.813	1437	1441	1445	rBV	1699089	1567603	60.64%	6.242%
18	11.519	1557	1561	1564	rBV	1194570	1014813	39.26%	4.041%
19	12.730	1765	1767	1770	rVB3	37878	34119	1.32%	0.136%
20	12.966	1804	1807	1808	rVB3	38554	29626	1.15%	0.118%
21	13.101	1826	1830	1834	rBV	2769228	2468276	95.48%	9.829%
22	13.319	1864	1867	1870	rVB5	51319	48426	1.87%	0.193%
23	13.507	1897	1899	1900	rBV2	30466	27603	1.07%	0.110%
24	13.660	1923	1925	1929	rVB5	61824	59441	2.30%	0.237%
25	13.983	1977	1980	1983	rVB2	182448	171077	6.62%	0.681%
26	14.166	2007	2011	2014	rBV	1269394	1174347	45.43%	4.676%
27	14.307	2033	2035	2039	rBV5	89882	78752	3.05%	0.314%
28	14.619	2085	2088	2094	rVB5	218854	226307	8.75%	0.901%
29	14.936	2140	2142	2145	rBV4	84209	86774	3.36%	0.346%
30	15.018	2154	2156	2160	rBV4	72906	68197	2.64%	0.272%
31	15.301	2202	2204	2206	rVB3	84139	49546	1.92%	0.197%
32	15.701	2267	2272	2276	rVB2	583856	740573	28.65%	2.949%

LSC Area Percent Report

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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-BF071618.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

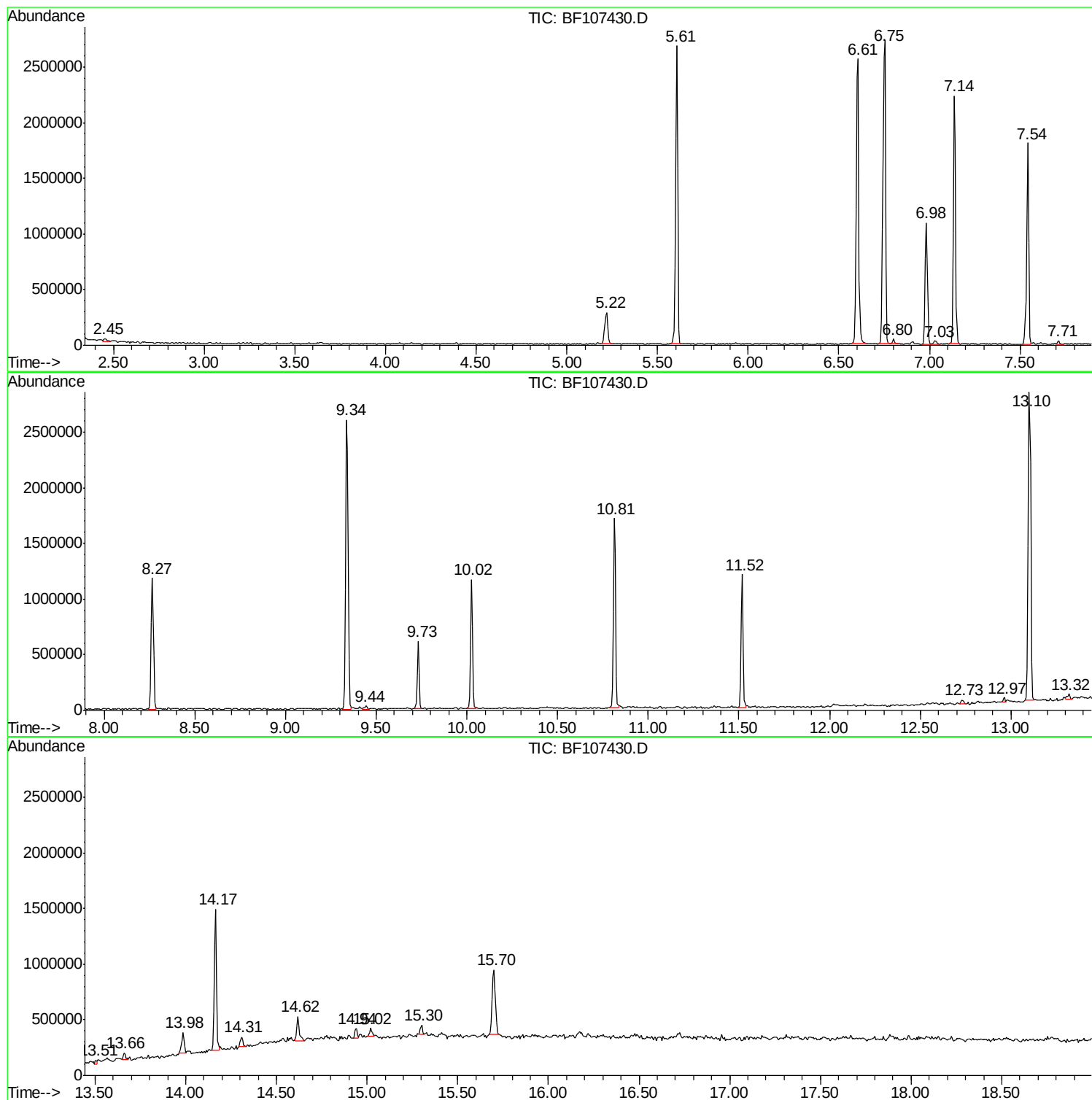
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF071618.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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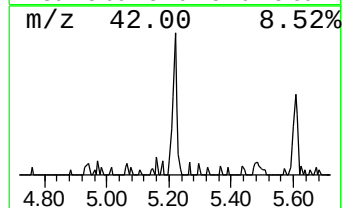
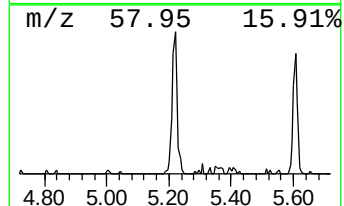
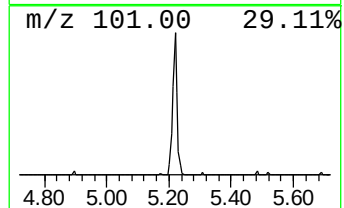
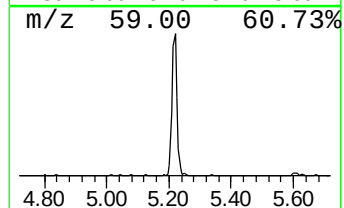
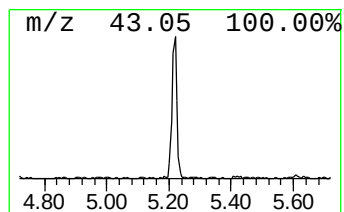
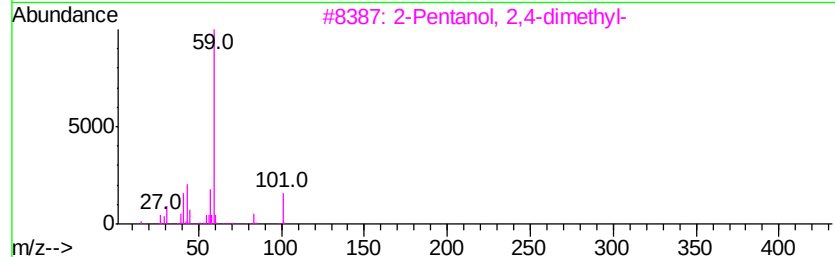
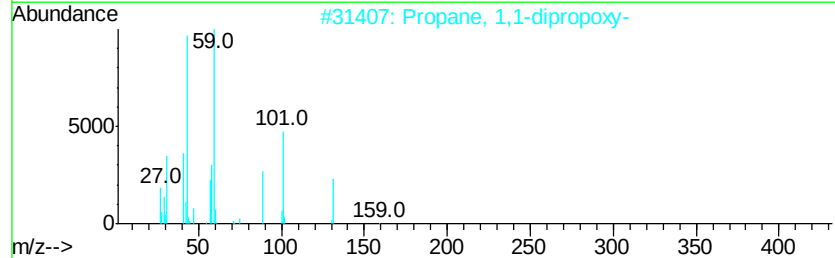
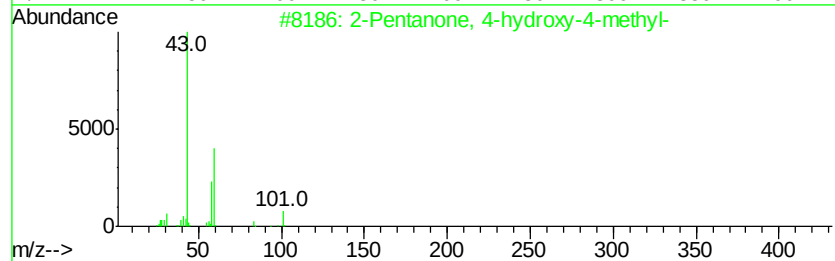
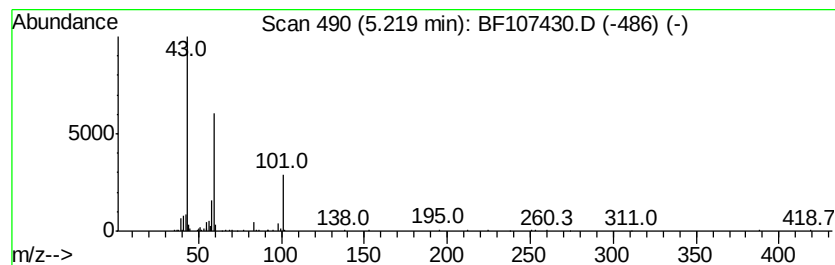
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.22	7.21 ng	313730	1,4-Dichlorobenzene-d4	6.98

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2			Propane, 1,1-dipropoxy-	160	C9H20O2	004744-11-0	45
3			2-Pentanol, 2,4-dimethyl-	116	C7H16O	000625-06-9	40
4			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	38
5			2,3-Dimethyloxirane-2-carboxylic...	130	C6H10O3	1000306-64-4	28



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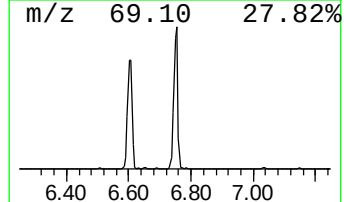
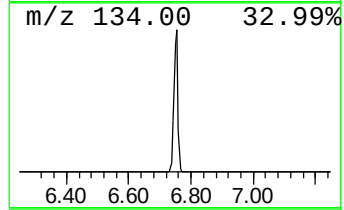
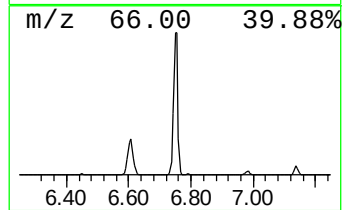
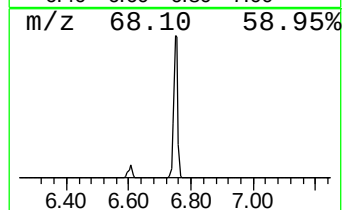
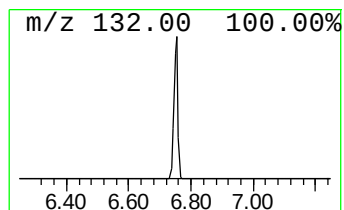
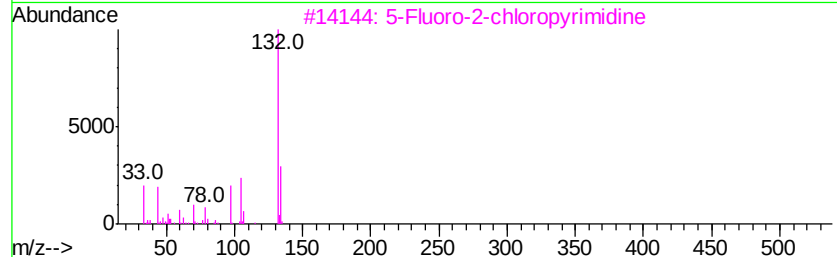
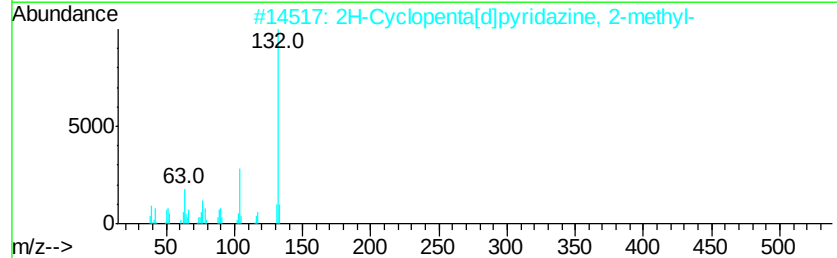
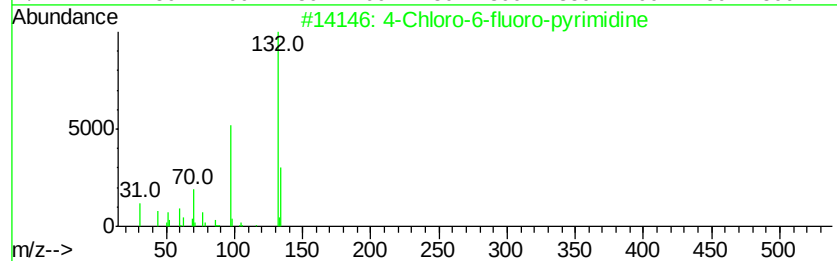
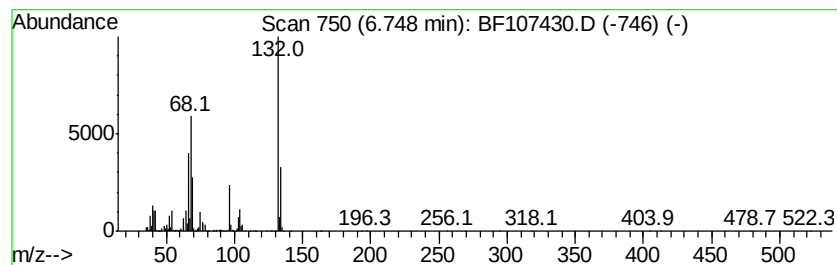
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 2 unknown6.75 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.75	59.39 ng	2585180	1,4-Dichlorobenzene-d4	6.98

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
2		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	22
3		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
4		Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	14
5		2-Cyclohexen-1-one	96	C6H8O	000930-68-7	10



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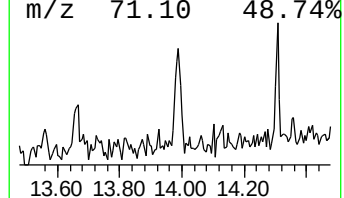
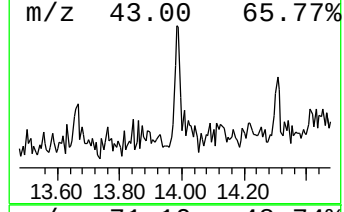
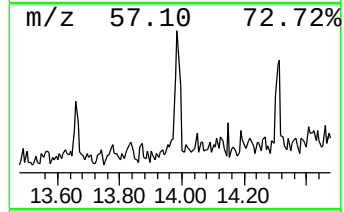
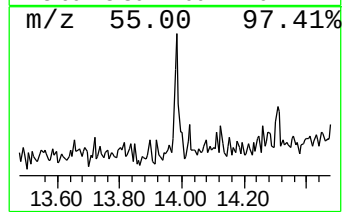
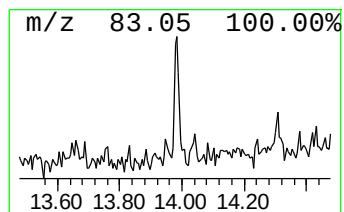
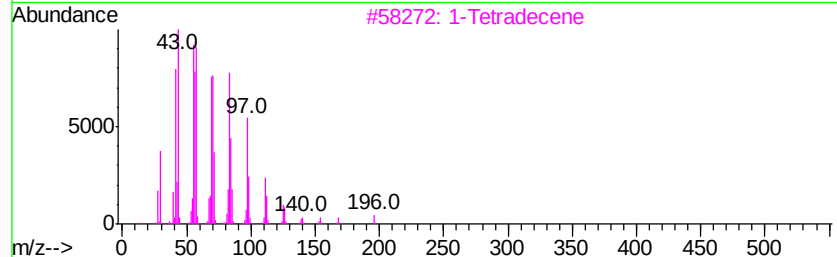
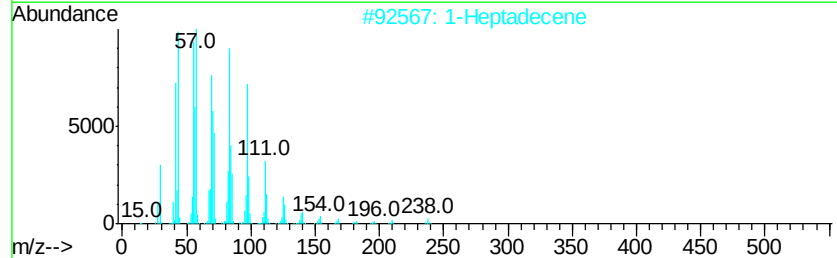
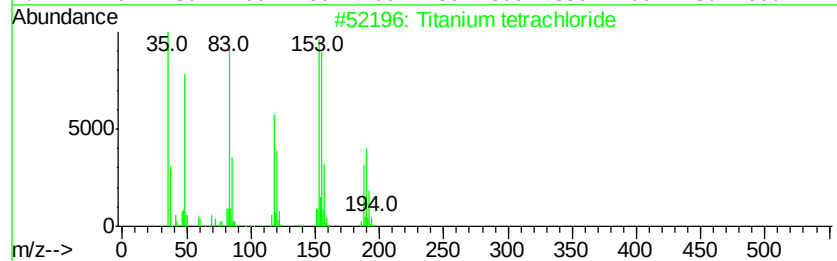
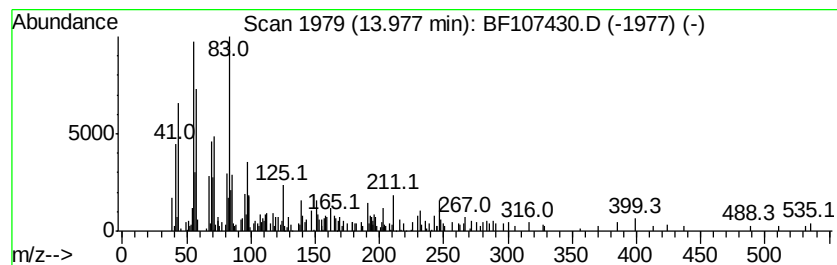
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Titanium tetrachloride Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.98	2.91 ng	171077	Chrysene-d12	14.17

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Titanium tetrachloride	188	Cl4Ti	007550-45-0	83
2		1-Heptadecene	238	C17H34	006765-39-5	83
3		1-Tetradecene	196	C14H28	001120-36-1	83
4		Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	76
5		Cyclohexane, (2-decyldodecyl)-	392	C28H56	006704-00-3	72



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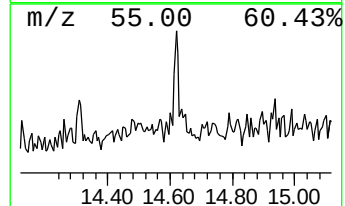
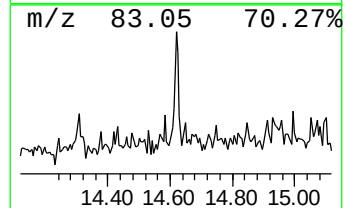
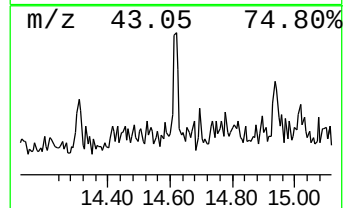
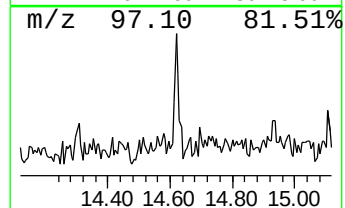
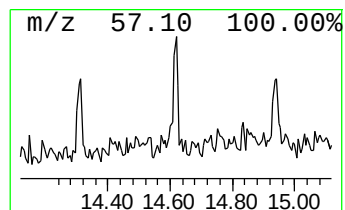
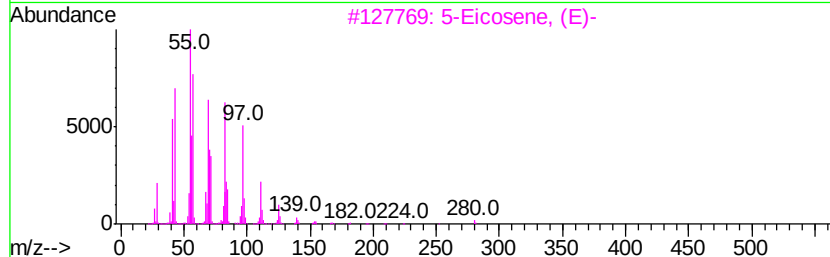
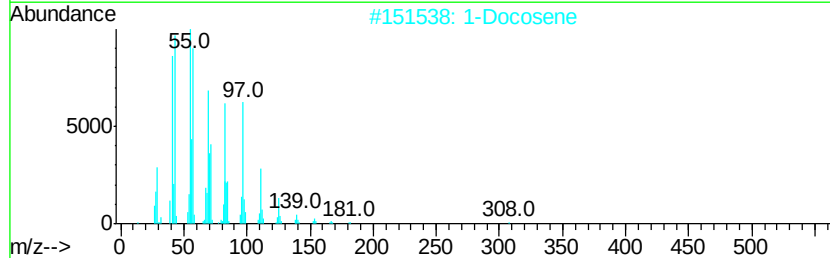
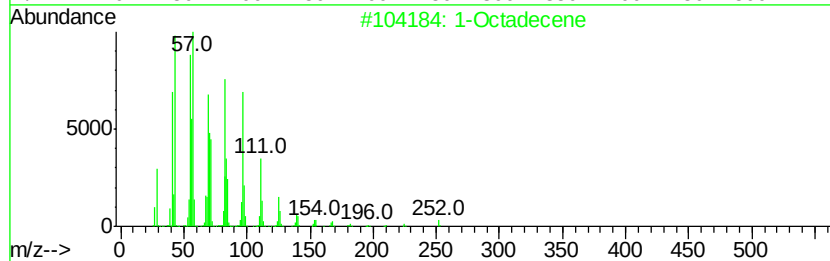
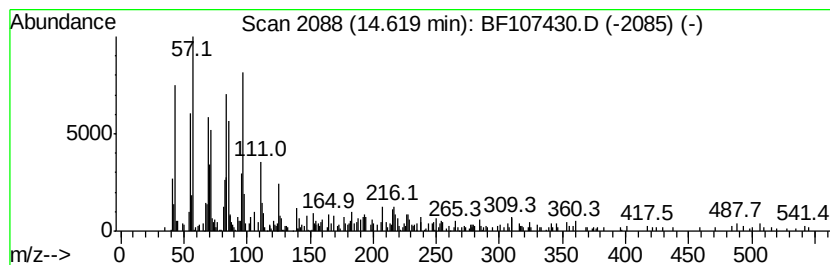
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 1-Octadecene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.62	3.85 ng	226307	Chrysene-d12	14.17

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Octadecene	252	C18H36	000112-88-9	86
2		1-Docosene	308	C22H44	001599-67-3	86
3		5-Eicosene, (E)-	280	C20H40	074685-30-6	86
4		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	70
5		1-Eicosene	280	C20H40	003452-07-1	70



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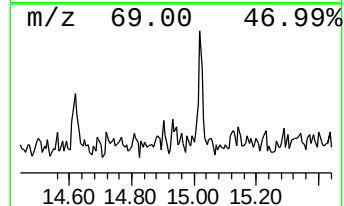
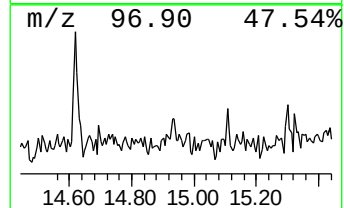
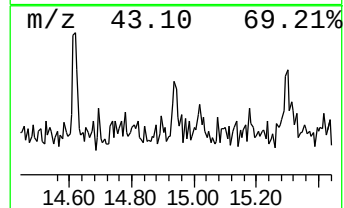
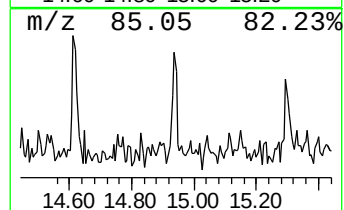
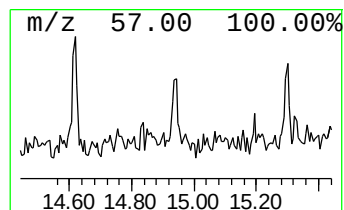
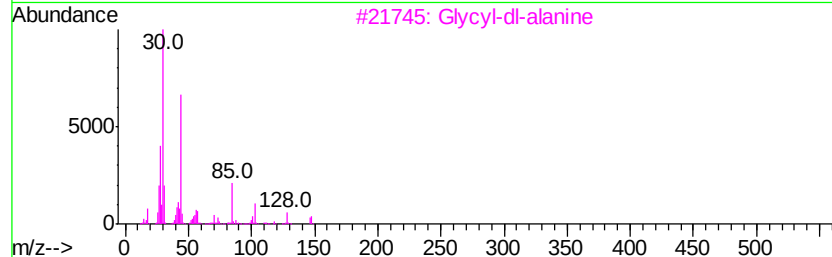
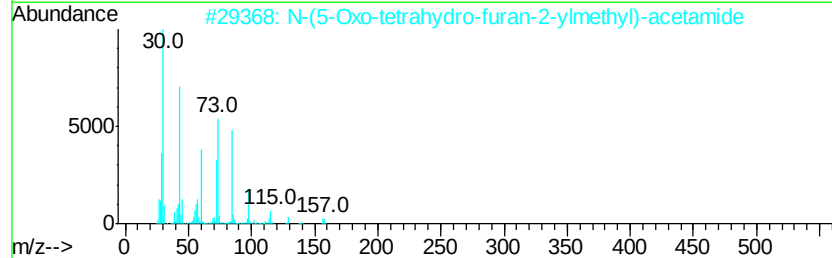
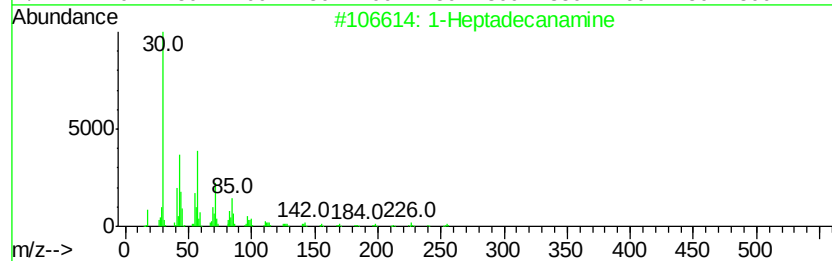
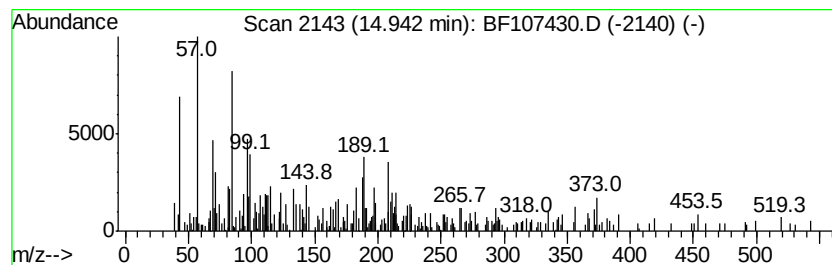
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Peak Number 6 1-Heptadecanamine Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.94	2.34 ng	86774	Perylene-d12	15.70

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Heptadecanamine	255	C17H37N	004200-95-7	7
2		N-(5-Oxo-tetrahydro-furan-2-ylme...	157	C7H11N03	1000188-71-2	4
3		Glycyl-dl-alanine	146	C5H10N2O3	000926-77-2	4
4		2,3-Octanedione	142	C8H14O2	000585-25-1	4
5		2,2,2-Trifluoroethylamine	99	C2H4F3N	000753-90-2	3



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Misc :
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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...	5.22	7.2	ng	313730	1	6.98	870516	20.0
unknown6.75	6.75	59.4	ng	2585180	1	6.98	870516	20.0
Titanium tetrachl...	13.98	2.9	ng	171077	5	14.17	1174350	20.0
1-Octadecene	14.62	3.9	ng	226307	5	14.17	1174350	20.0
1-Heptadecanamine	14.94	2.3	ng	86774	6	15.70	740573	20.0