

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF111219\
 Data File : BF117763.D
 Acq On : 12 Nov 2019 16:55
 Operator : JU
 Sample : K5789-11
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP-16B-D

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-BF110619.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	2.216	17	22	39	rVB	1302743	1848611	31.82%	3.451%
2	5.140	514	519	526	rVB	908426	1112001	19.14%	2.076%
3	5.540	582	587	590	rBV	5266694	5009326	86.22%	9.353%
4	6.545	752	758	762	rBV	5121157	5360029	92.25%	10.007%
5	6.692	778	783	786	rBV	5781723	5360008	92.25%	10.007%
6	6.928	819	823	826	rVB	1808600	1615344	27.80%	3.016%
7	7.081	845	849	853	rBV	4916801	4234178	72.87%	7.905%
8	7.487	913	918	921	rBV	3468902	3290125	56.63%	6.143%
9	8.210	1037	1041	1045	rBV	2507039	2085118	35.89%	3.893%
10	9.286	1220	1224	1228	rBV	5951136	5810256	100.00%	10.848%
11	9.681	1287	1291	1294	rBV	696372	518849	8.93%	0.969%
12	9.975	1336	1341	1344	rBV	2572874	2309062	39.74%	4.311%
13	10.763	1470	1475	1478	rBV	3706423	3470484	59.73%	6.480%
14	11.463	1590	1594	1598	rBV	2612959	2125318	36.58%	3.968%
15	11.533	1600	1606	1609	rVB2	66799	73369	1.26%	0.137%
16	11.986	1679	1683	1688	rBV	335406	321432	5.53%	0.600%
17	12.774	1813	1817	1822	rBV	71924	89931	1.55%	0.168%
18	13.051	1860	1864	1868	rBV	4919069	4713109	81.12%	8.800%
19	13.957	2014	2018	2035	rVB	204581	431256	7.42%	0.805%
20	14.110	2040	2044	2048	rBV	1718704	1601024	27.56%	2.989%
21	14.980	2189	2192	2198	rVB	127447	133566	2.30%	0.249%
22	15.257	2236	2239	2245	rVB	66397	89405	1.54%	0.167%
23	15.621	2296	2301	2306	rBV	1543272	1900091	32.70%	3.548%
24	15.657	2306	2307	2312	rVB	60570	58555	1.01%	0.109%

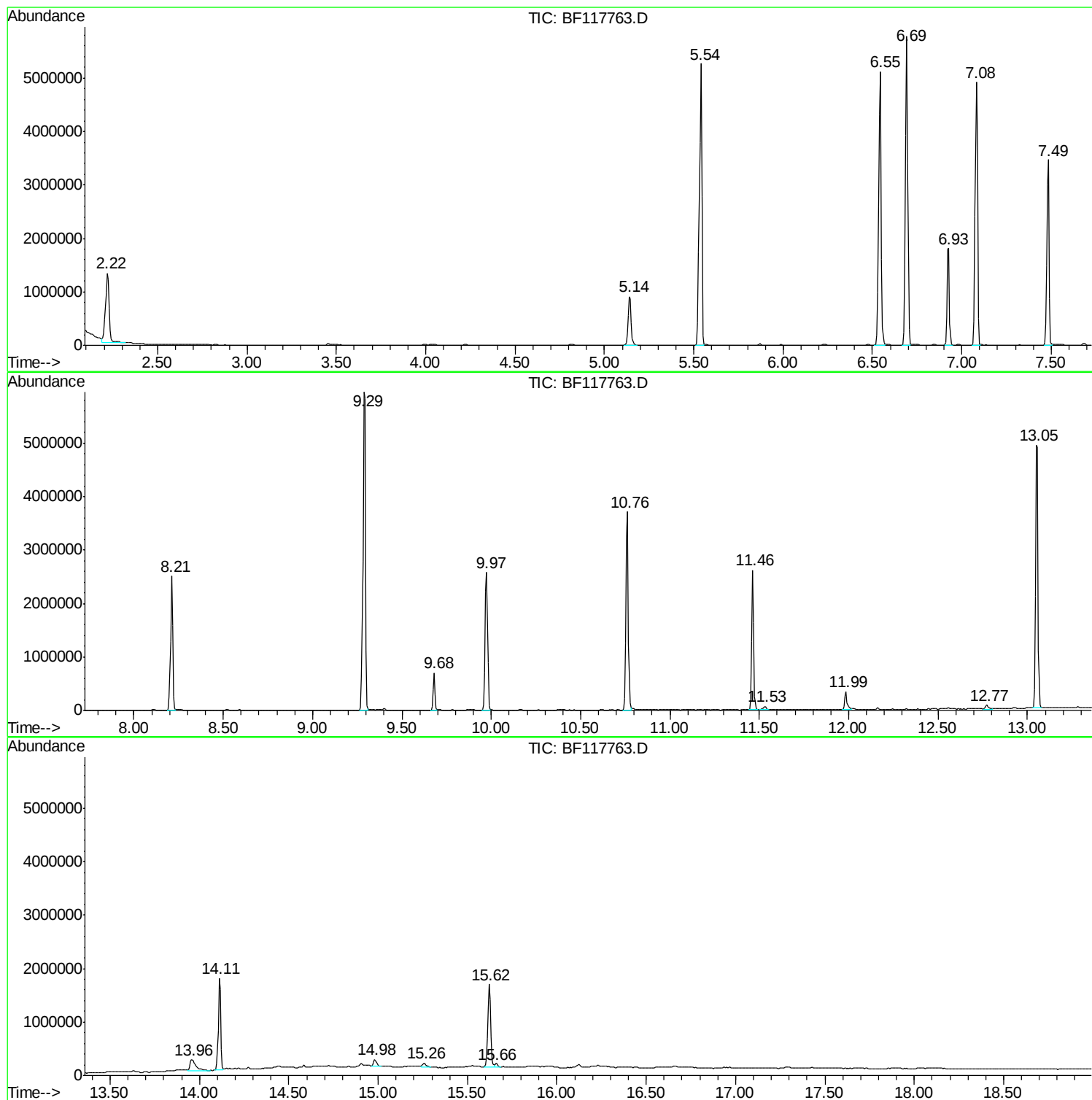
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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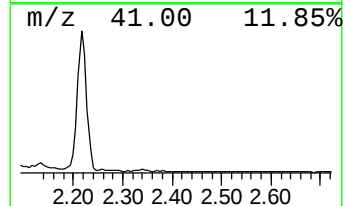
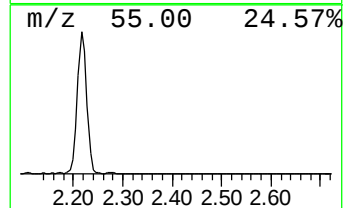
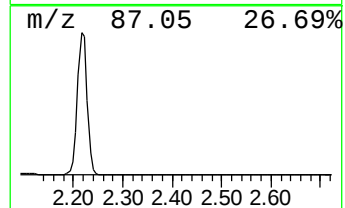
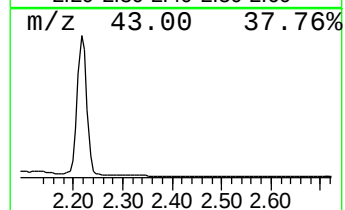
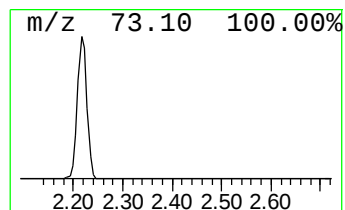
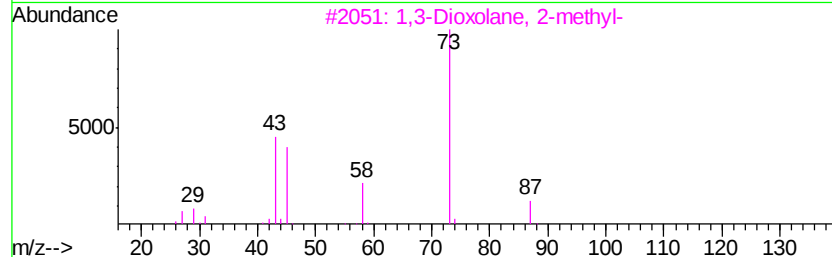
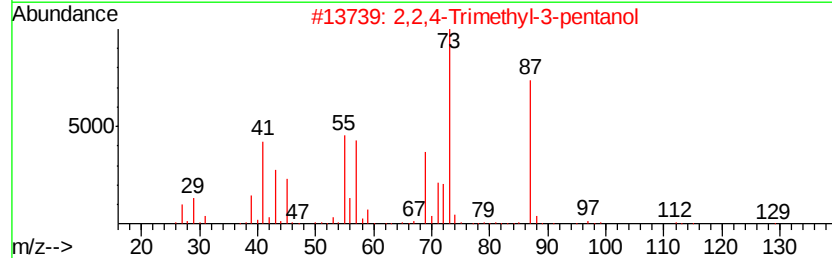
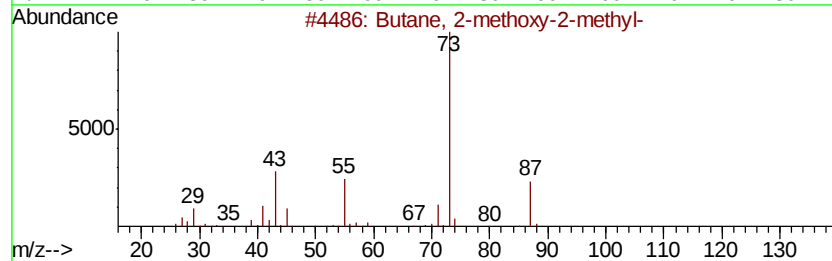
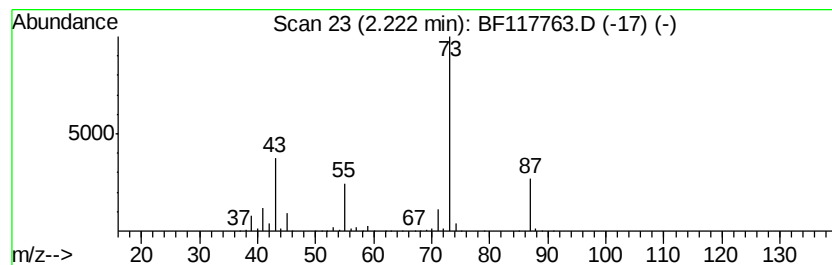
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.22	22.89 ng	1848610	1,4-Dichlorobenzene-d4	6.93

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
4		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
5		Silane, tetramethyl-	88	C4H12Si	000075-76-3	10



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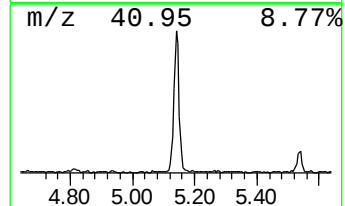
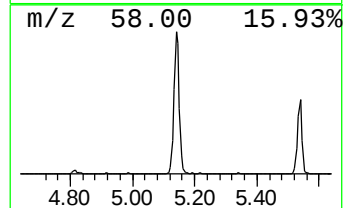
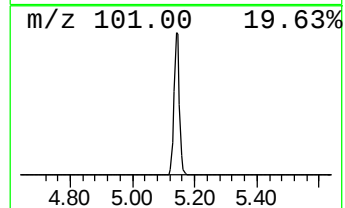
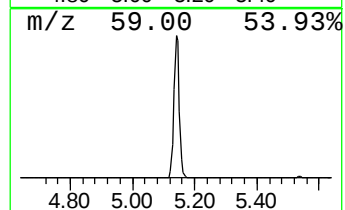
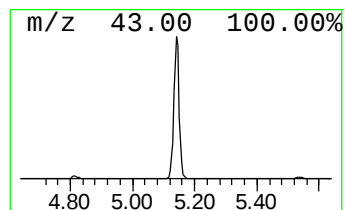
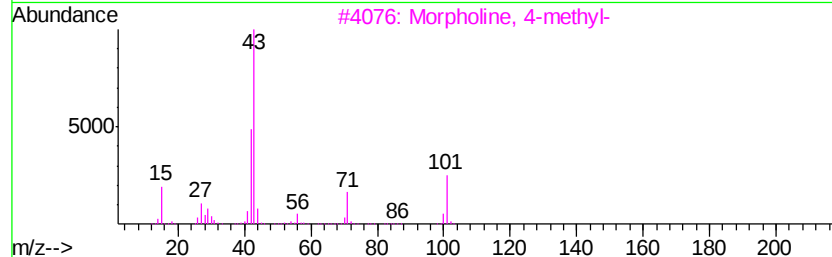
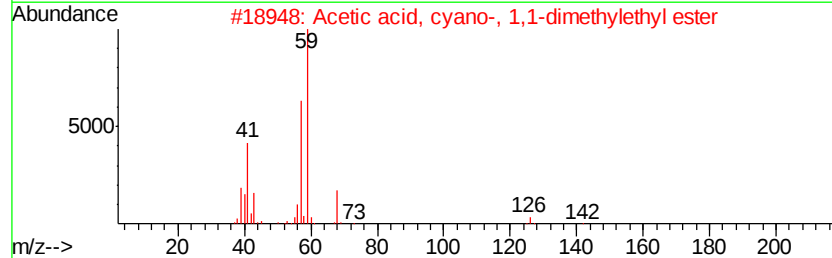
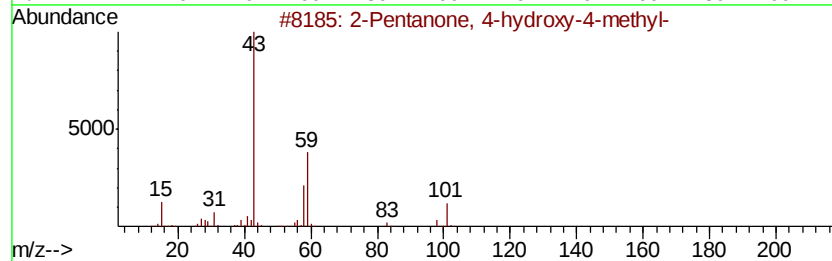
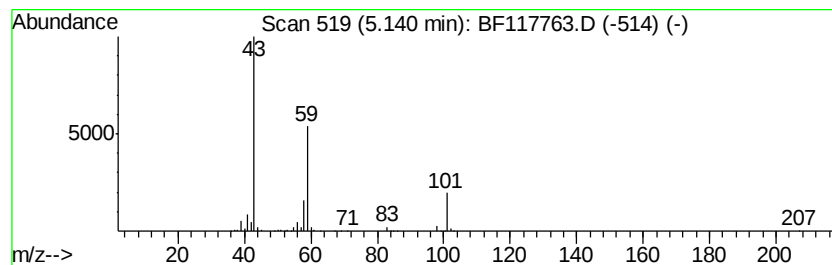
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.14	13.77 ng	1112000	1,4-Dichlorobenzene-d4	6.93

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	25
3		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4		Propanoic acid, 2-nitro-, methyl...	133	C4H7NO4	006118-50-9	9
5		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	9



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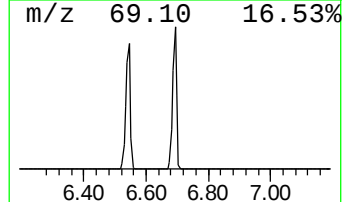
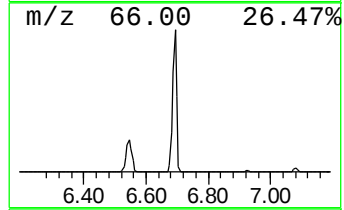
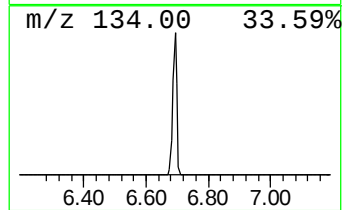
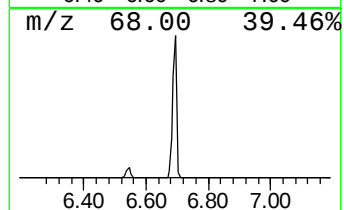
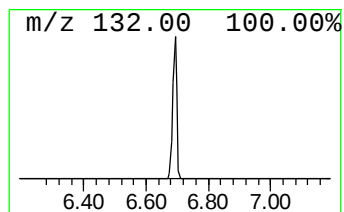
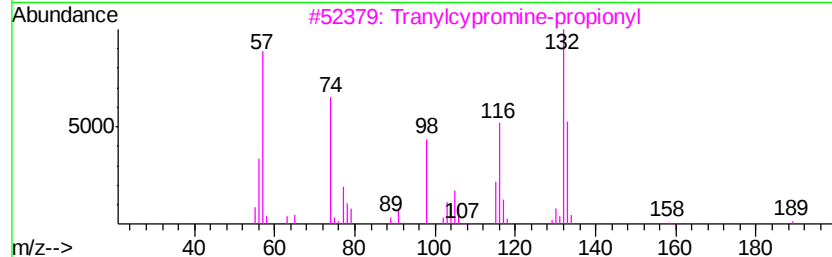
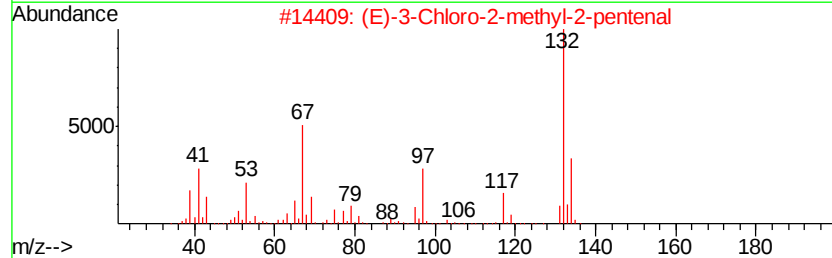
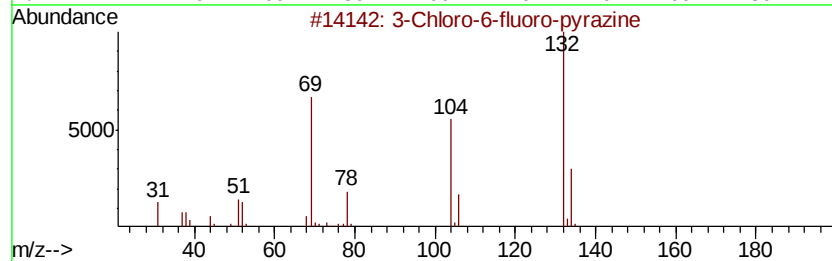
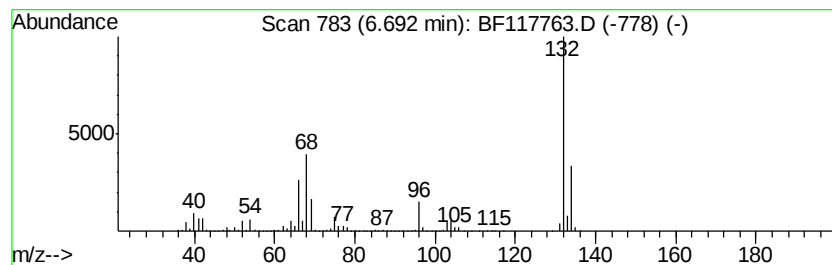
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Peak Number 3 unknown6.69 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.69	66.36 ng	5360010	1,4-Dichlorobenzene-d4	6.93

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	16
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	12
4		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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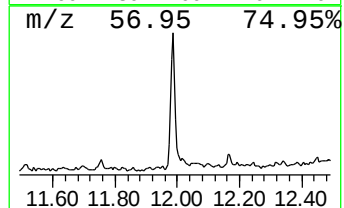
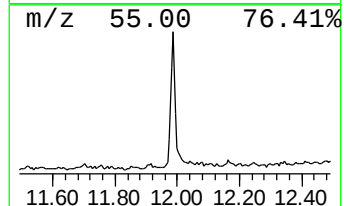
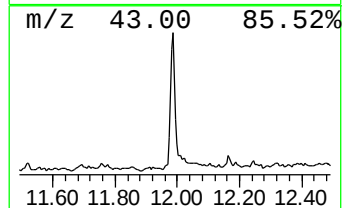
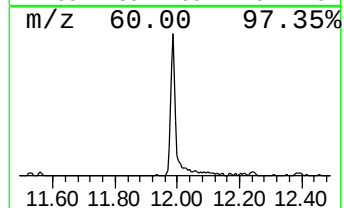
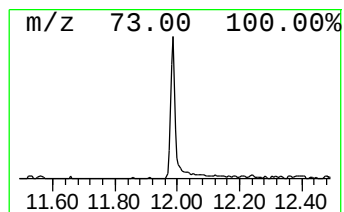
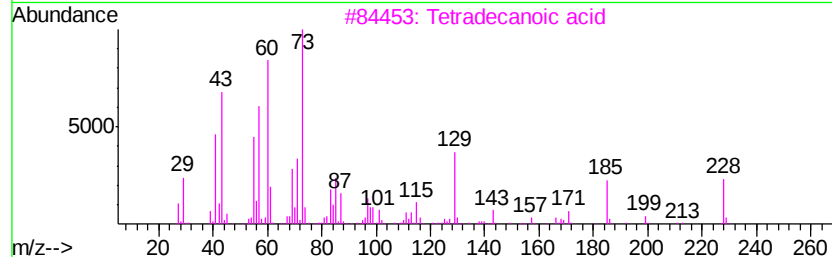
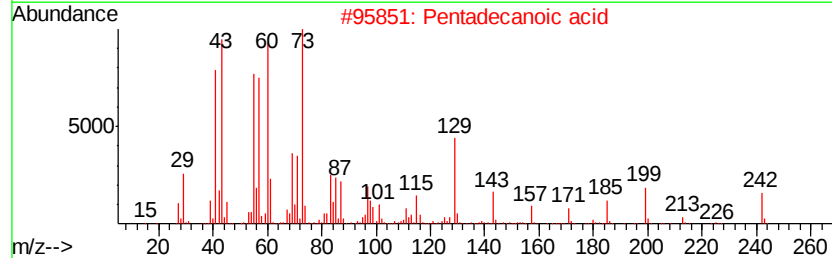
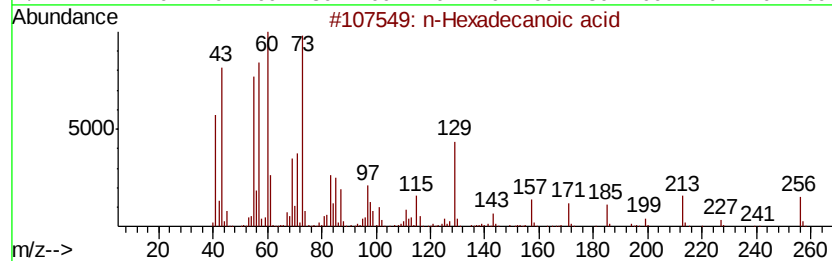
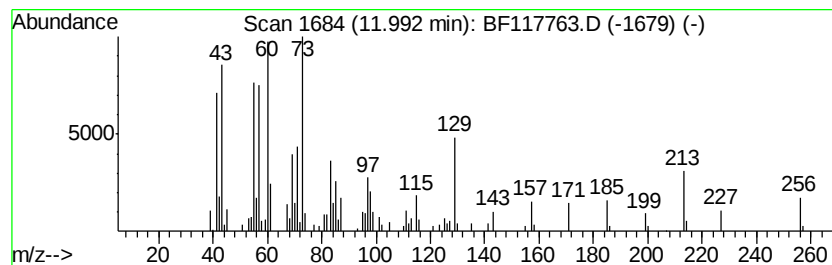
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Peak Number 5 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.99	3.02 ng	321432	Phenanthrene-d10	11.46

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	91
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	81
4		Tridecanoic acid	214	C13H26O2	000638-53-9	76
5		n-Decanoic acid	172	C10H20O2	000334-48-5	70



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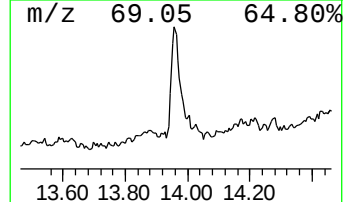
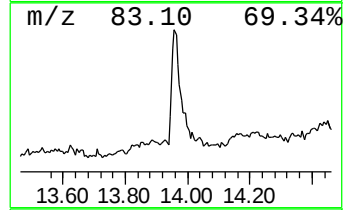
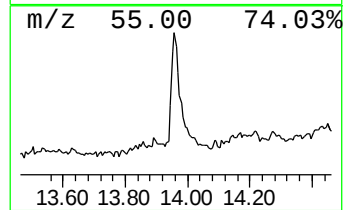
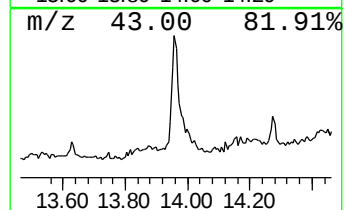
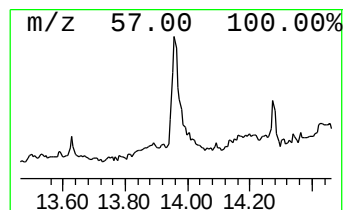
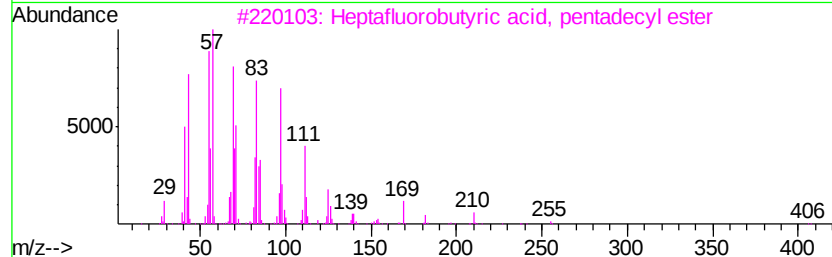
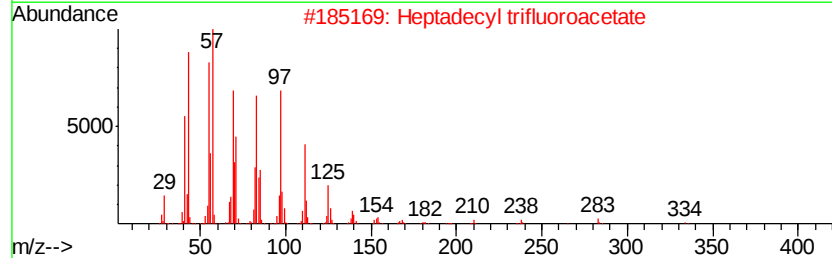
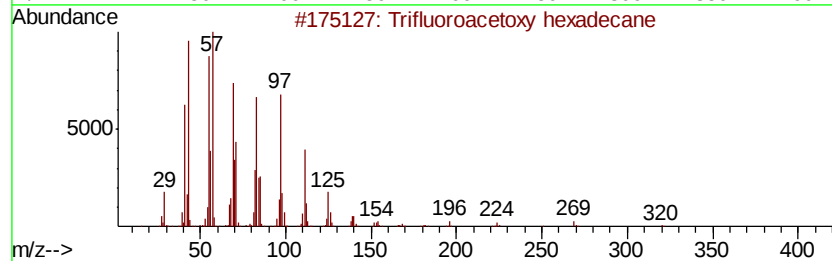
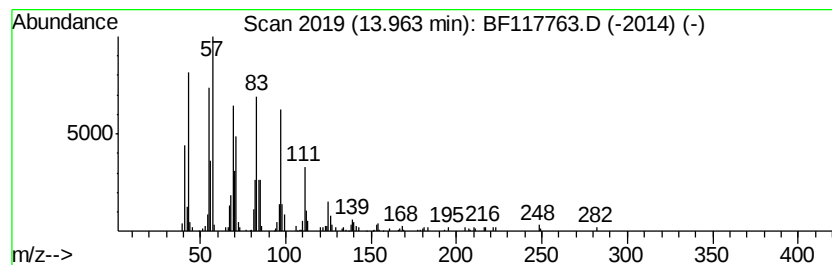
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TIC Integration Parameters: LSCINT.P

Peak Number 6 Trifluoroacetoxy hexadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.96	5.39 ng	431256	Chrysene-d12	14.11

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	95
2		Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	94
3		Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94
4		Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
5		Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	91



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-methoxy...	2.22	22.9	ng	1848610	1	6.93	1615340	20.0
2-Pentanone, 4-hy...	5.14	13.8	ng	1112000	1	6.93	1615340	20.0
unknown6.69	6.69	66.4	ng	5360010	1	6.93	1615340	20.0
n-Hexadecanoic acid	11.99	3.0	ng	321432	4	11.46	2125320	20.0
Trifluoroacetoxy ...	13.96	5.4	ng	431256	5	14.11	1601020	20.0