

Data Path : Z:\HPCHEM1\BNA F\DATA\BF080717\
 Data File : BF097460.D
 Acq On : 8 Aug 2017 6:28
 Operator : SJ/JU
 Sample : I4628-01
 Misc :
 ALS Vial : 34 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 RW-3

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:\HPCHEM1\BNA_F\METHODS\8270-BF072517.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	4.534	463	467	475	rBV	45624	82966	3.68%	0.489%
2	5.004	544	547	567	rBV	899331	1270133	56.35%	7.485%
3	6.081	727	730	744	rBV	655706	937747	41.60%	5.526%
4	6.187	744	748	758	rVB	2112317	2254121	100.00%	13.284%
5	6.410	783	786	798	rVB	560109	529521	23.49%	3.120%
6	6.569	809	813	829	rVB	1918076	1967653	87.29%	11.595%
7	6.987	880	884	901	rBV	1736378	1824823	80.95%	10.754%
8	7.692	1001	1004	1014	rBV	739708	666846	29.58%	3.930%
9	8.004	1050	1057	1059	rBV3	13381	24123	1.07%	0.142%
10	8.310	1104	1109	1115	rBV6	18315	38185	1.69%	0.225%
11	8.357	1115	1117	1120	rVB	36331	31447	1.40%	0.185%
12	8.492	1137	1140	1146	rBV3	24925	36865	1.64%	0.217%
13	8.775	1183	1188	1191	rBV	2270576	2159578	95.81%	12.726%
14	8.875	1199	1205	1206	rBV4	25208	34466	1.53%	0.203%
15	9.045	1229	1234	1237	rBV4	21181	41803	1.85%	0.246%
16	9.175	1253	1256	1259	rBV	54062	48032	2.13%	0.283%
17	9.245	1264	1268	1273	rBV6	15897	28591	1.27%	0.168%
18	9.433	1297	1300	1310	rBV	577698	561920	24.93%	3.311%
19	9.892	1376	1378	1381	rVB2	26107	22755	1.01%	0.134%
20	10.045	1401	1404	1409	rBV	20503	26109	1.16%	0.154%
21	10.228	1431	1435	1446	rBV	1016347	1104917	49.02%	6.511%
22	10.363	1455	1458	1462	rBV2	36504	43191	1.92%	0.255%
23	10.910	1547	1551	1557	rBV	507853	438579	19.46%	2.585%
24	10.992	1561	1565	1569	rVB6	13457	22790	1.01%	0.134%
25	11.027	1569	1571	1578	rBV7	20054	40628	1.80%	0.239%
26	11.475	1643	1647	1652	rBV2	50529	70159	3.11%	0.413%
27	12.251	1776	1779	1785	rBV	35276	43238	1.92%	0.255%
28	12.492	1816	1820	1824	rBV	1687769	1724614	76.51%	10.163%
29	13.427	1976	1979	1986	rVB8	22218	33703	1.50%	0.199%
30	13.533	1993	1997	2004	rVB	500214	460142	20.41%	2.712%
31	14.604	2172	2179	2183	rBV8	20942	50466	2.24%	0.297%
32	14.874	2221	2225	2229	rBV	290958	323943	14.37%	1.909%
33	15.257	2286	2290	2296	rBV6	13324	25174	1.12%	0.148%

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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

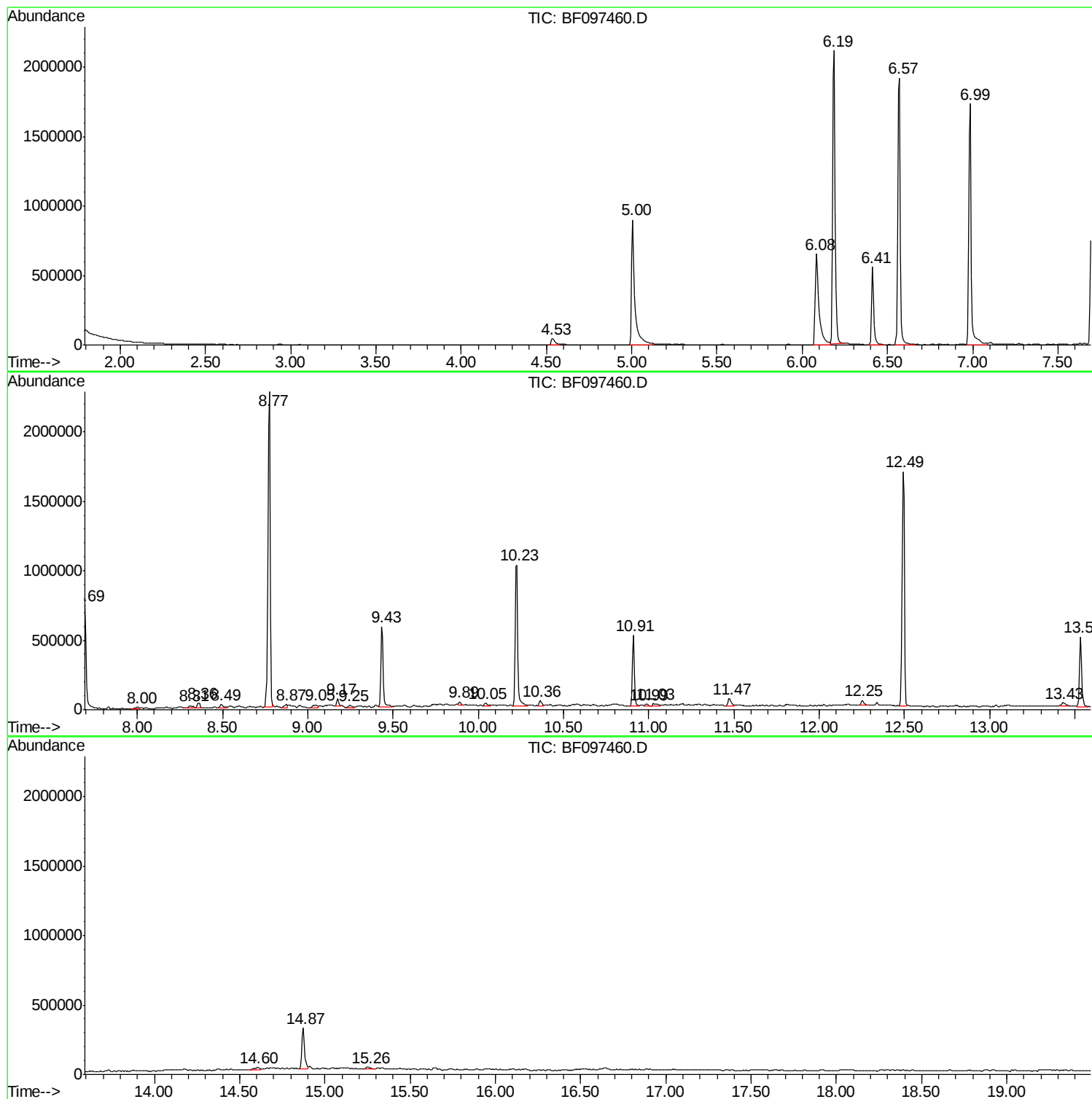
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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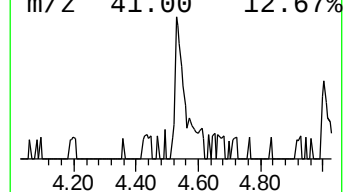
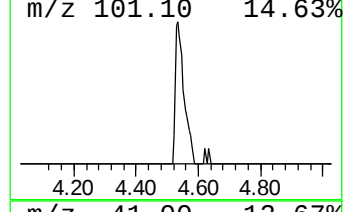
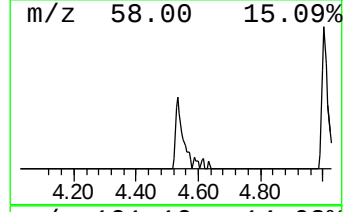
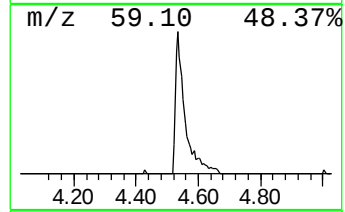
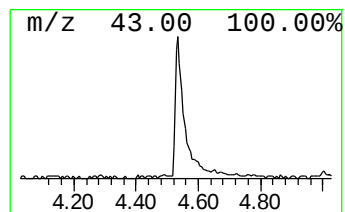
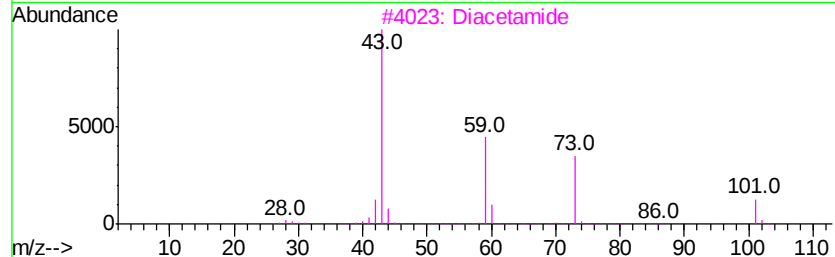
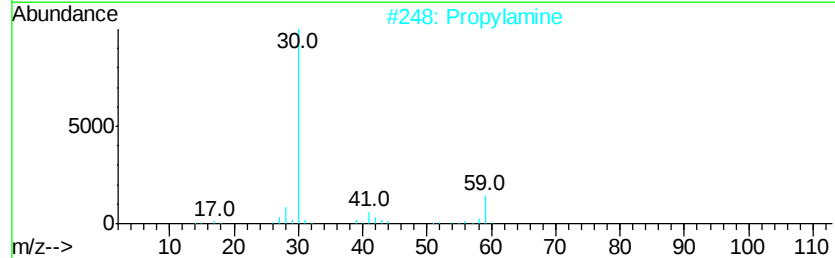
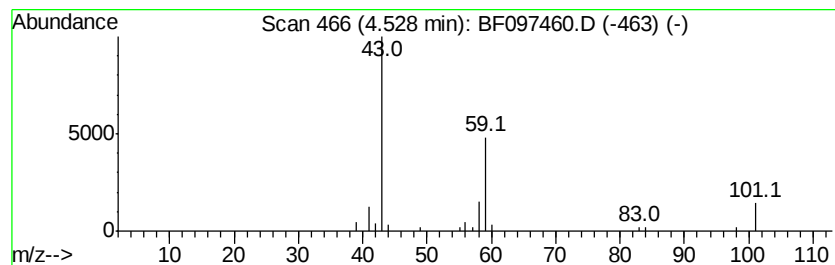
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.53	3.13 ng	82966	1,4-Dichlorobenzene-d4	6.41

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2			Propylamine	59	C3H9N	000107-10-8	9
3			Diacetamide	101	C4H7NO2	000625-77-4	9
4			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9
5			3-Octanol	130	C8H18O	000589-98-0	9



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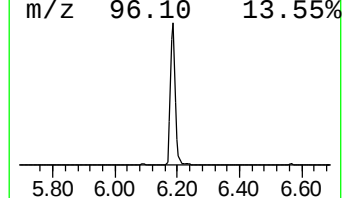
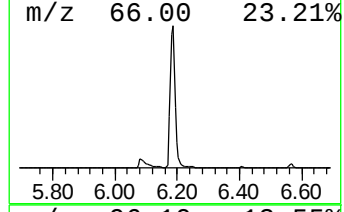
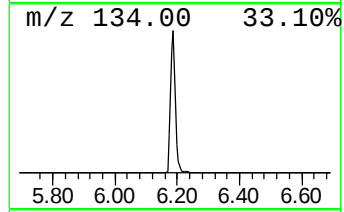
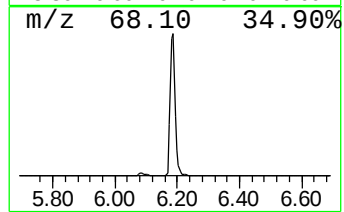
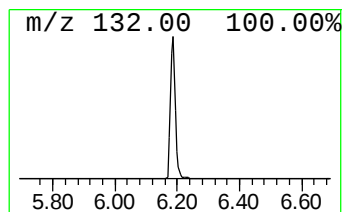
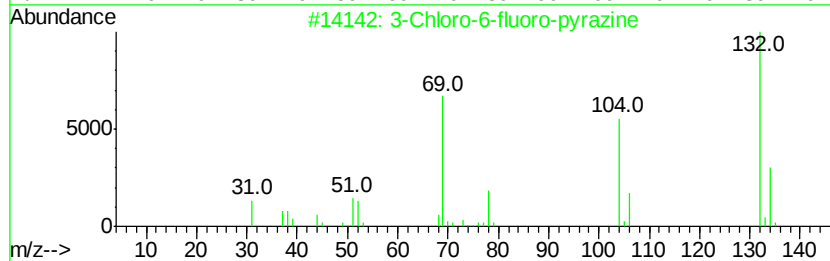
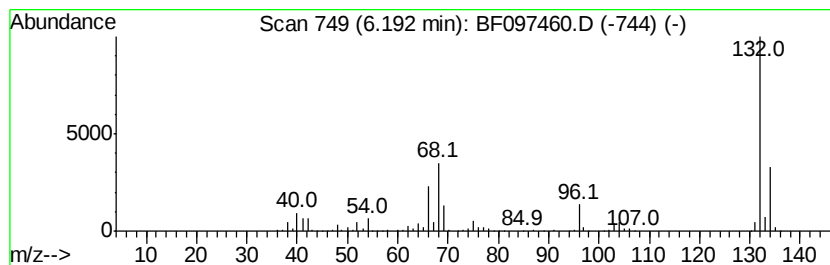
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown6.19 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.19	85.14 ng	2254120	1,4-Dichlorobenzene-d4	6.41

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	17
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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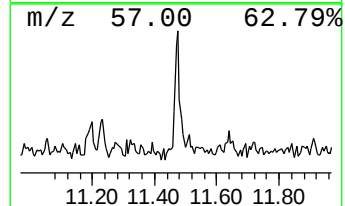
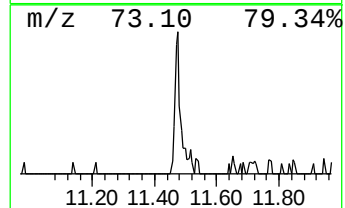
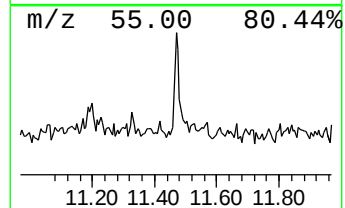
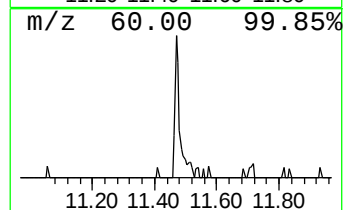
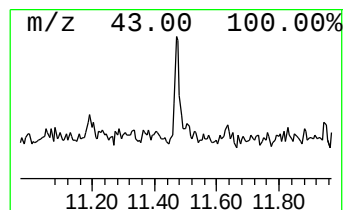
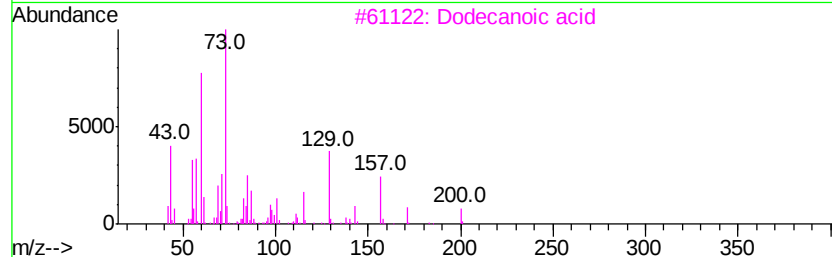
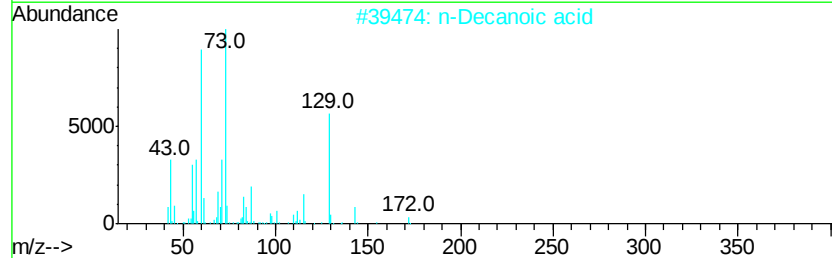
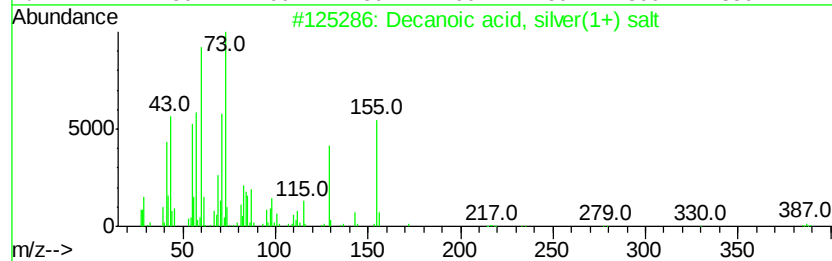
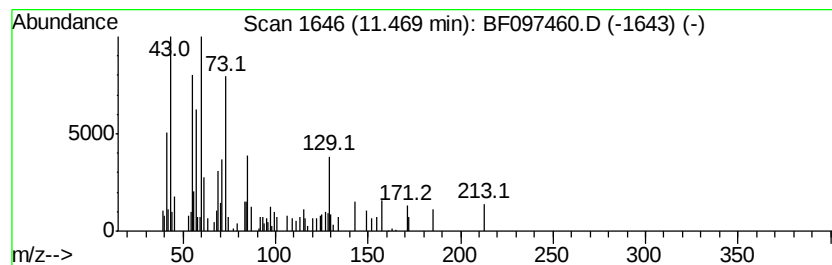
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Peak Number 4 Decanoic acid, silver(1+) salt Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.47	3.20 ng	70159	Phenanthrene-d10	10.91

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	58
2		n-Decanoic acid	172	C10H20O2	000334-48-5	53
3		Dodecanoic acid	200	C12H24O2	000143-07-7	43
4		3,5-Difluorobenzaldehyde carbamo...	199	C8H7F2N3O	163893-49-0	30
5		Octane, 3,4,5,6-tetramethyl-	170	C12H26	062185-21-1	10



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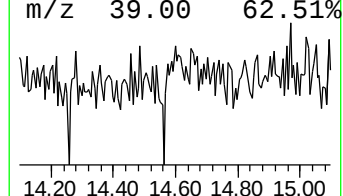
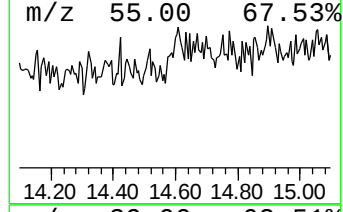
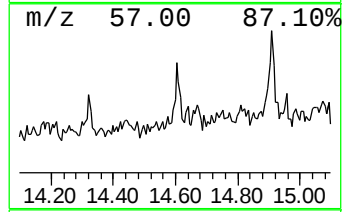
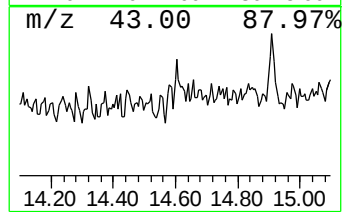
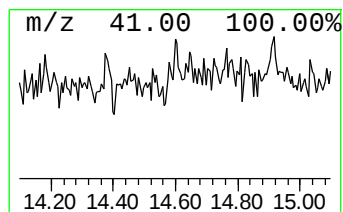
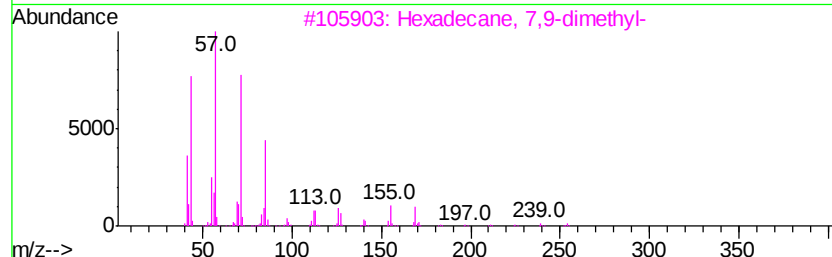
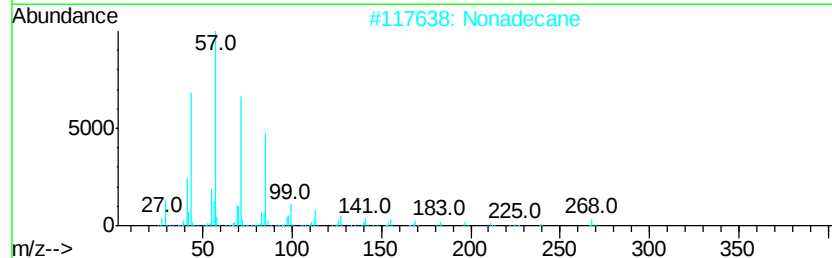
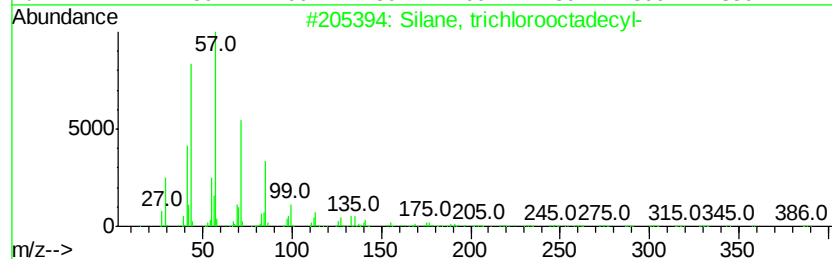
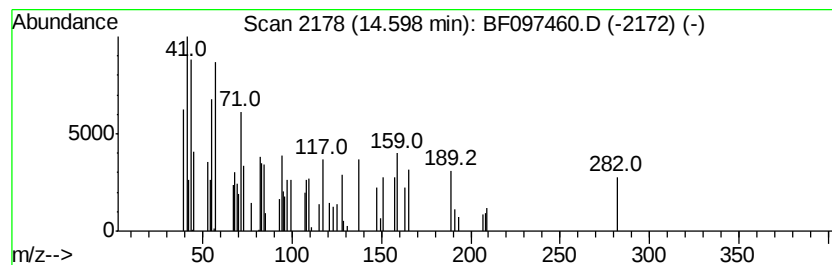
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 unknown14.60 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.60	3.12 ng	50466	Perylene-d12	14.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Silane, trichlorooctadecyl-	386	C18H37Cl3Si	000112-04-9	38
2		Nonadecane	268	C19H40	000629-92-5	35
3		Hexadecane, 7,9-dimethyl-	254	C18H38	021164-95-4	35
4		Heptadecane	240	C17H36	000629-78-7	35
5		Pentadecane	212	C15H32	000629-62-9	35



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.53	3.1	ng	82966	1	6.41	529521	20.0
unknown6.19	6.19	85.1	ng	2254120	1	6.41	529521	20.0
Decanoic acid, si...	11.47	3.2	ng	70159	4	10.91	438579	20.0
unknown14.60	14.60	3.1	ng	50466	6	14.87	323943	20.0