

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF073116\
Data File : BF089476.D
Acq On : 31 Jul 2016 17:49
Operator : UM/SJ
Sample : H4257-06
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TEC-COMP-6

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:\HPCHEM1\BNA_F\METHODS\8270-BF072716.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	1.656	5	6	50	rVB	800746	2066863	100.00%	15.898%
2	4.582	259	262	273	rBV	287411	523754	25.34%	4.029%
3	5.062	302	304	330	rBV	1019667	1233001	59.66%	9.484%
4	5.473	338	340	346	rVB	23610	28158	1.36%	0.217%
5	6.159	397	400	402	rBV	923368	1237914	59.89%	9.522%
6	6.262	407	409	411	rBV	1233097	1308759	63.32%	10.067%
7	6.490	427	429	440	rVB	199249	231099	11.18%	1.778%
8	6.650	440	443	445	rBV	671441	910677	44.06%	7.005%
9	7.062	477	479	490	rBV	523102	747069	36.15%	5.746%
10	7.782	540	542	553	rBV	207145	310125	15.00%	2.385%
11	8.856	634	636	639	rBV	1305450	1260416	60.98%	9.695%
12	9.256	669	671	674	rBV	218783	194060	9.39%	1.493%
13	9.519	692	694	697	rBV	407669	357394	17.29%	2.749%
14	10.308	761	763	765	rBV	719310	765881	37.06%	5.891%
15	10.445	773	775	779	rBV	26257	29429	1.42%	0.226%
16	10.994	821	823	838	rBV	285218	316053	15.29%	2.431%
17	11.554	869	872	875	rBV	15699	28543	1.38%	0.220%
18	12.194	926	928	931	rBV	34811	32249	1.56%	0.248%
19	12.422	945	948	951	rVB	19396	27549	1.33%	0.212%
20	12.571	959	961	964	rBV	842551	810199	39.20%	6.232%
21	13.485	1038	1041	1045	rBV2	21844	39374	1.91%	0.303%
22	13.611	1049	1052	1058	rBV	187603	233976	11.32%	1.800%
23	14.525	1130	1132	1135	rBV	36053	32706	1.58%	0.252%
24	14.605	1136	1139	1144	rBV	16000	32878	1.59%	0.253%
25	14.937	1166	1168	1174	rVB	195101	221028	10.69%	1.700%
26	15.143	1184	1186	1189	rBV	19392	21935	1.06%	0.169%

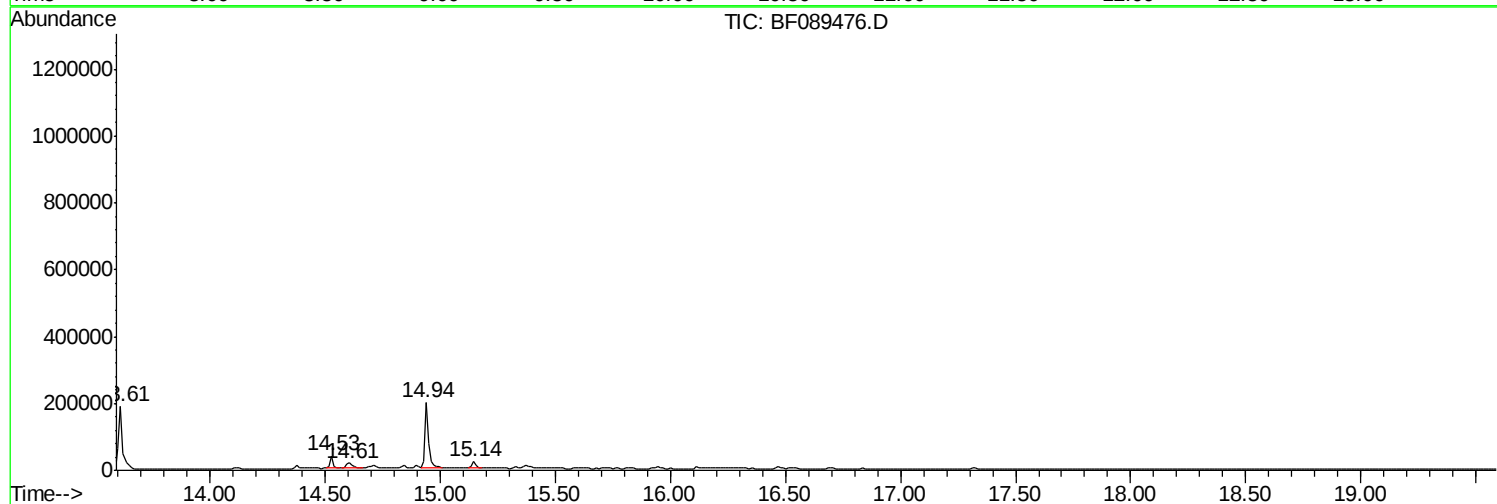
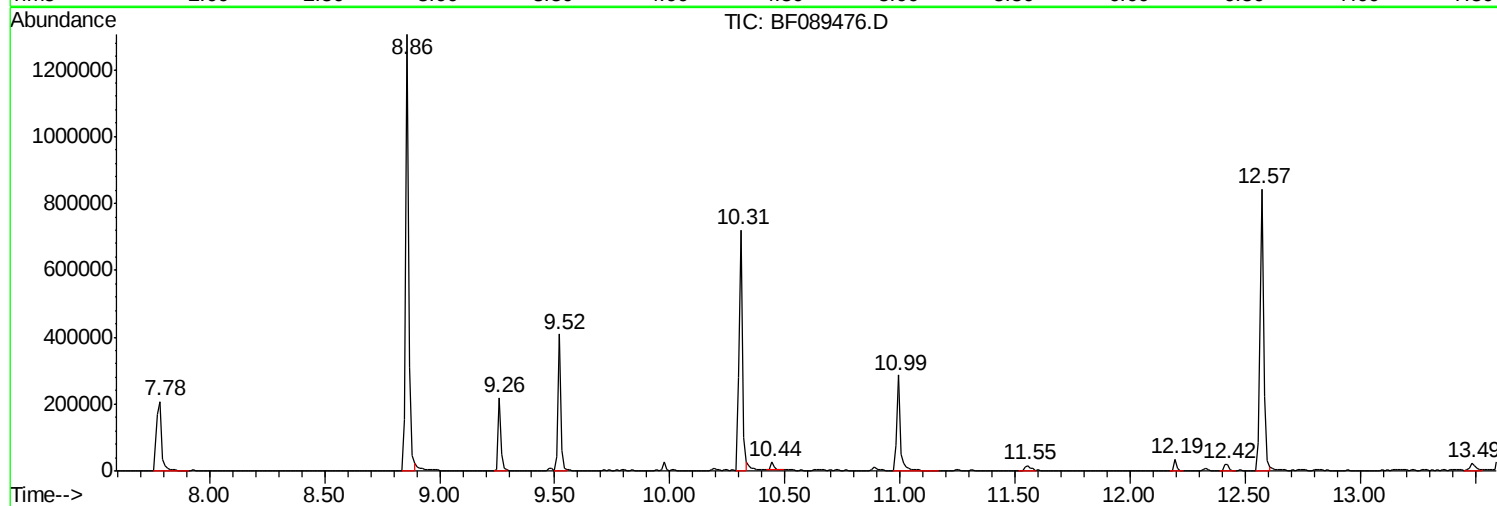
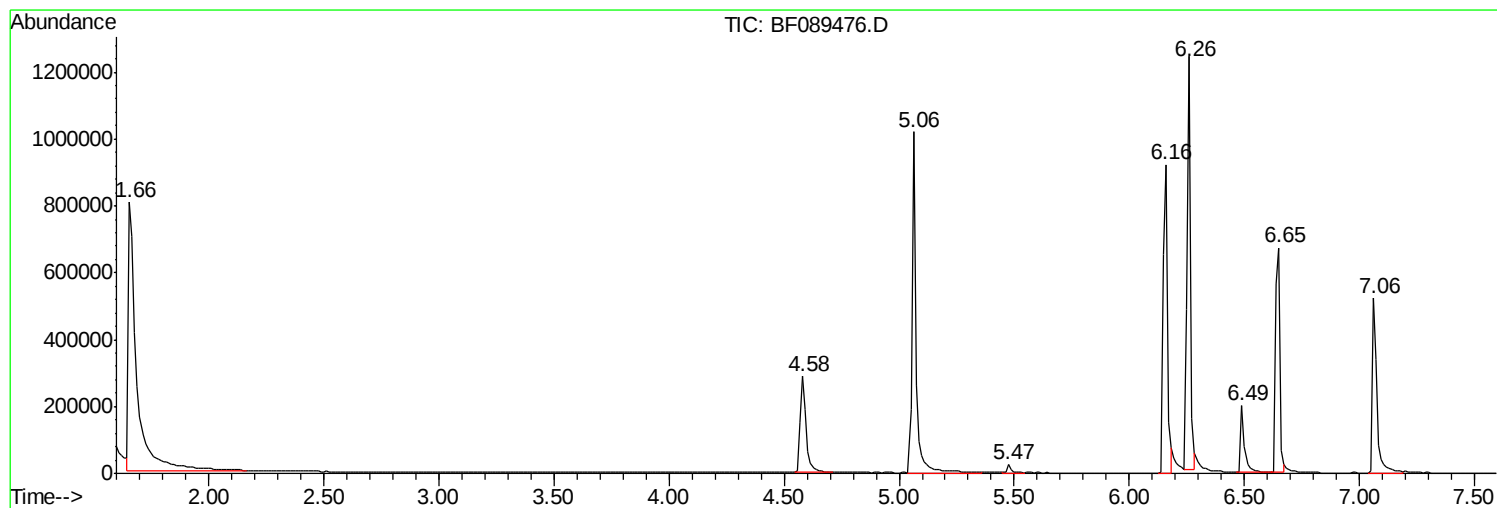
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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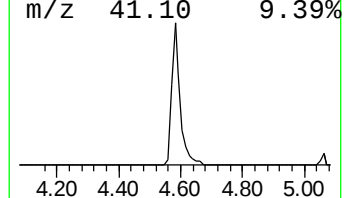
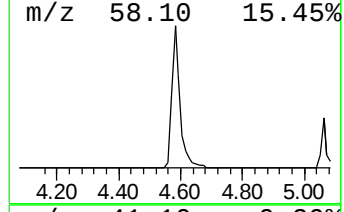
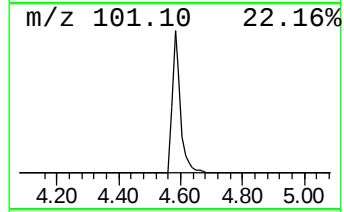
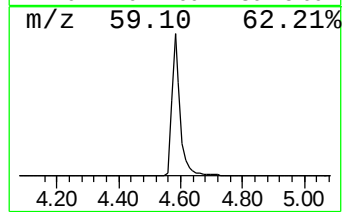
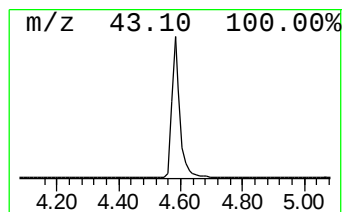
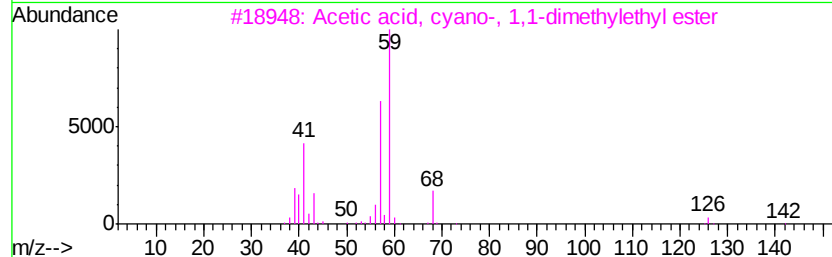
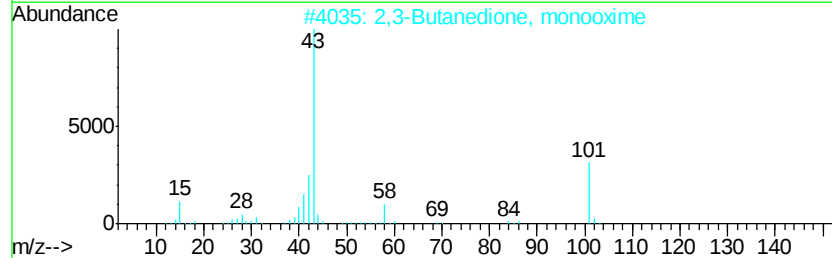
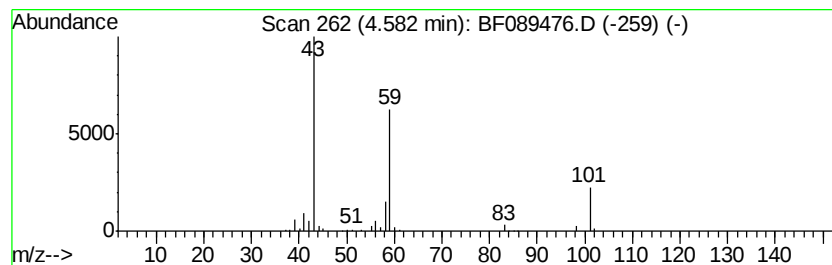
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.58	45.33 ng	523754	1,4-Dichlorobenzene-d4	6.49

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
3		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	23
4		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9



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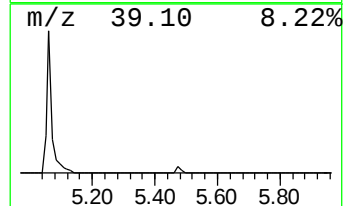
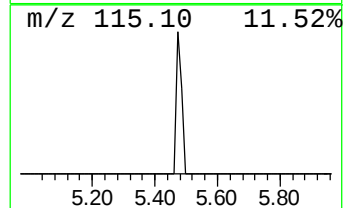
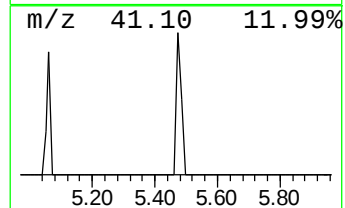
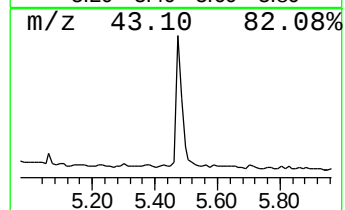
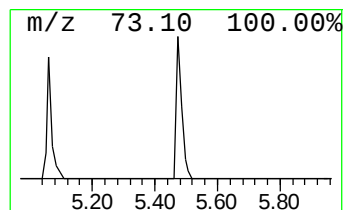
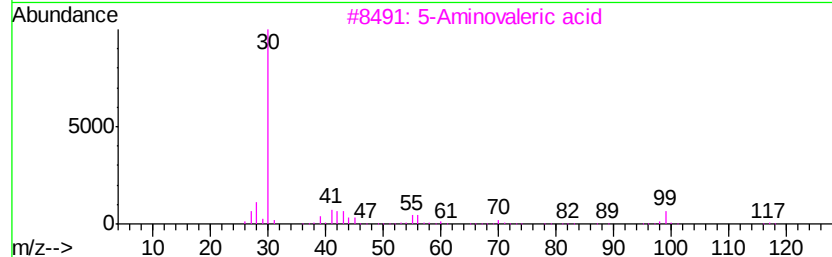
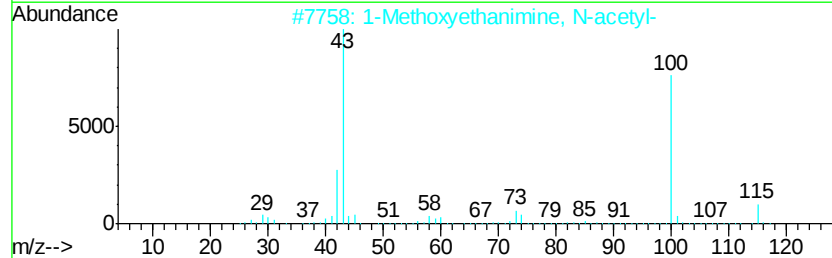
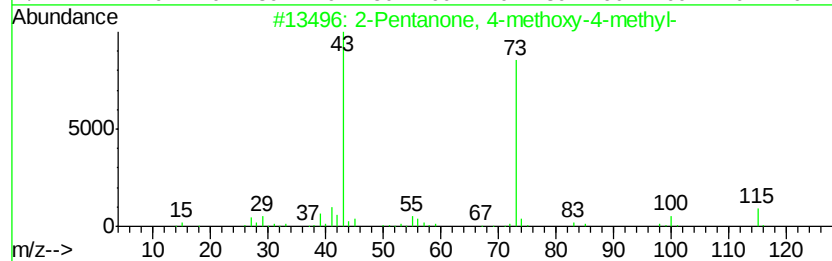
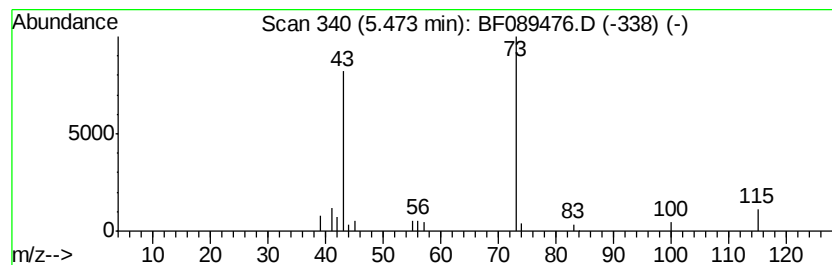
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Peak Number 3 2-Pentanone, 4-methoxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.47	2.44 ng	28158	1,4-Dichlorobenzene-d4	6.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	72
2	1-Methoxyethanimine, N-acetyl-	115	C5H9NO2	099028-43-0	9
3	5-Aminovaleric acid	117	C5H11NO2	000660-88-8	9
4	1-Propanol, 2-methyl-	74	C4H10O	000078-83-1	9
5	Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	9



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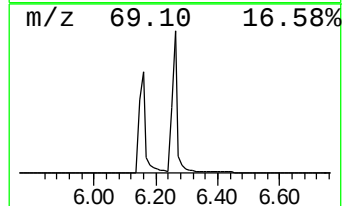
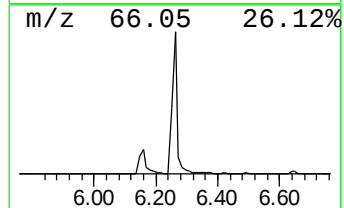
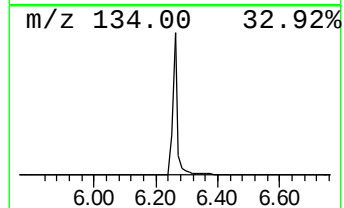
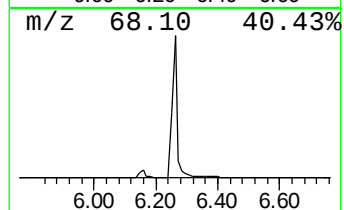
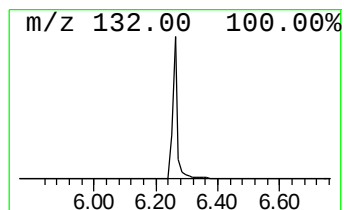
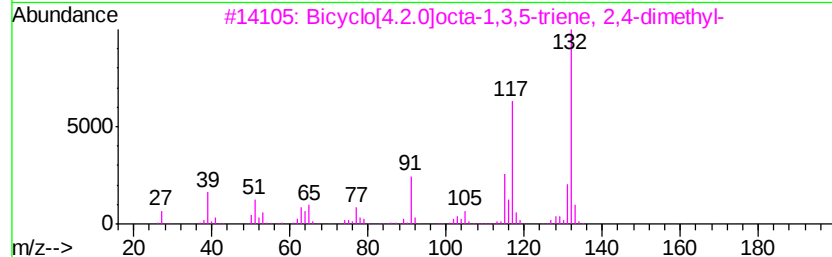
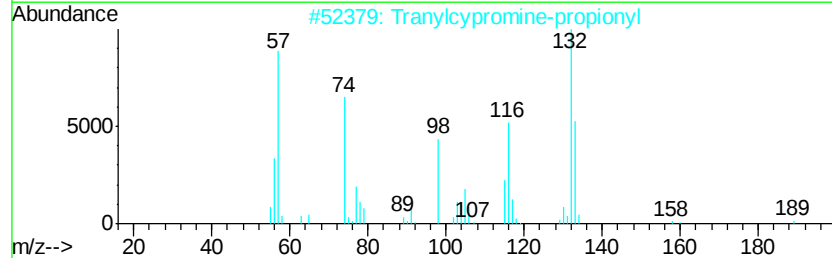
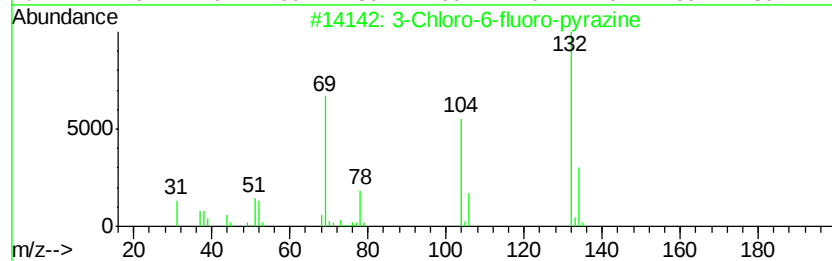
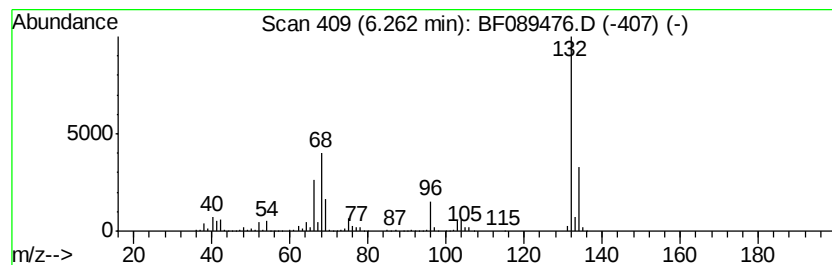
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Peak Number 4 unknown6.26 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.26	113.26 ng	1308760	1,4-Dichlorobenzene-d4	6.49

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9



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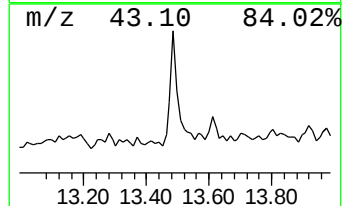
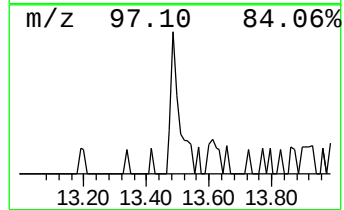
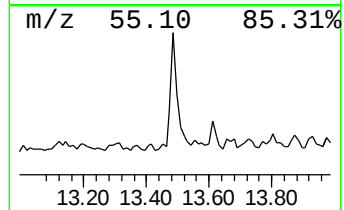
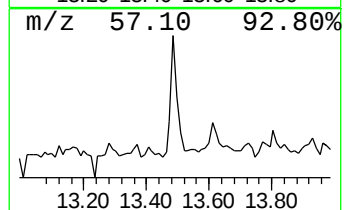
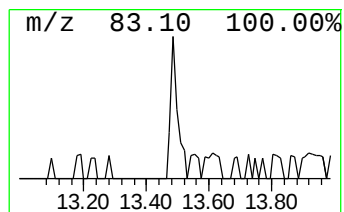
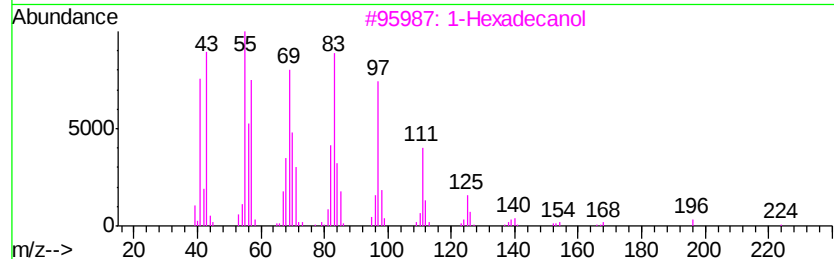
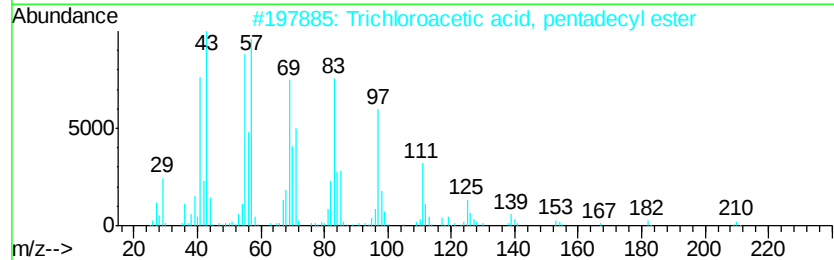
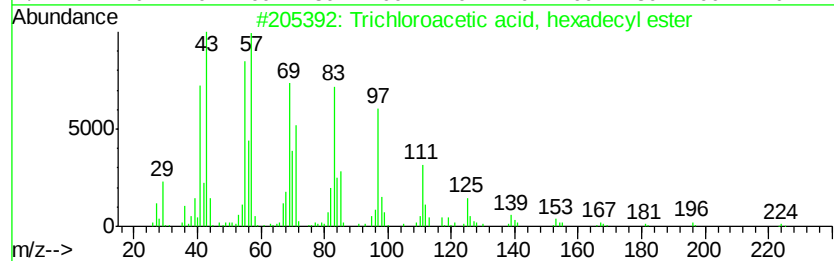
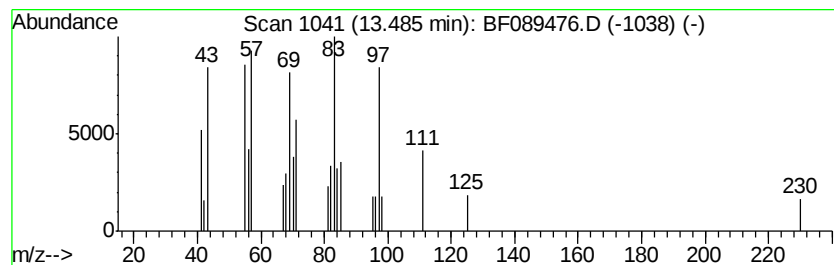
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TIC Library : C:\Database\NIST11.L
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Peak Number 6 Trichloroacetic acid, hexad... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.49	3.37 ng	39374	Chrysene-d12	13.61

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
2		Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	91
3		1-Hexadecanol	242	C16H34O	036653-82-4	90
4		n-Heptadecanol-1	256	C17H36O	001454-85-9	90
5		n-Nonadecanol-1	284	C19H40O	001454-84-8	90



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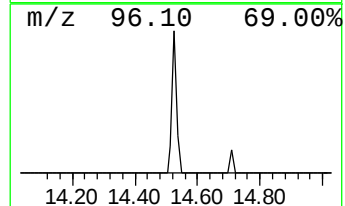
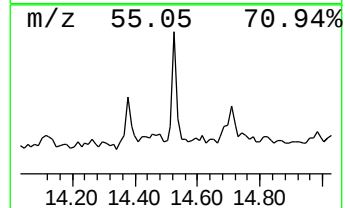
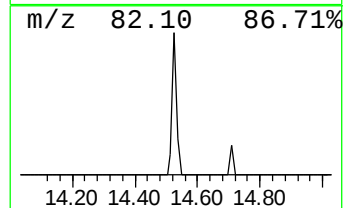
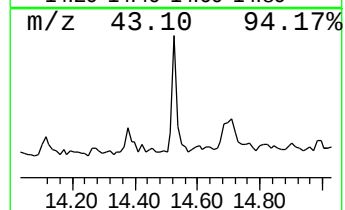
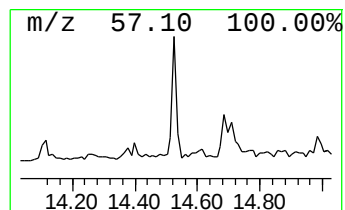
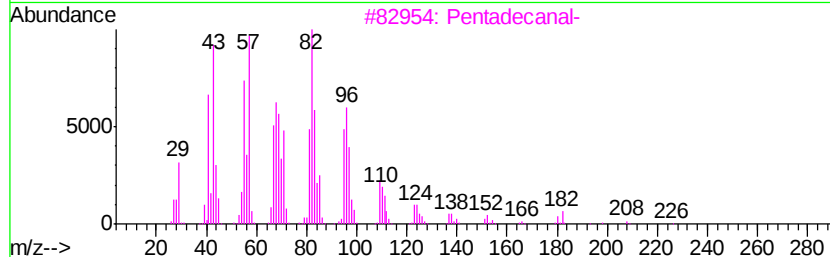
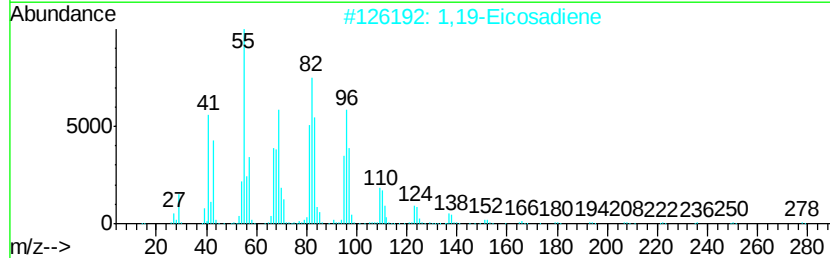
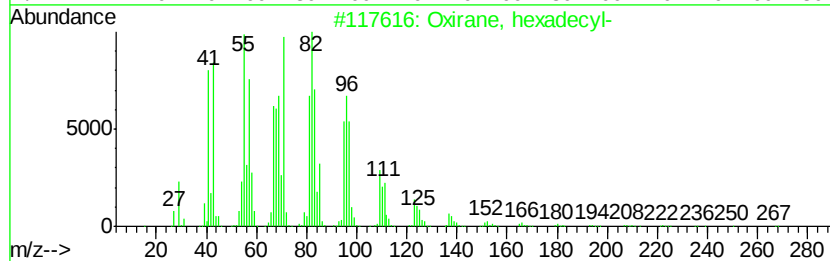
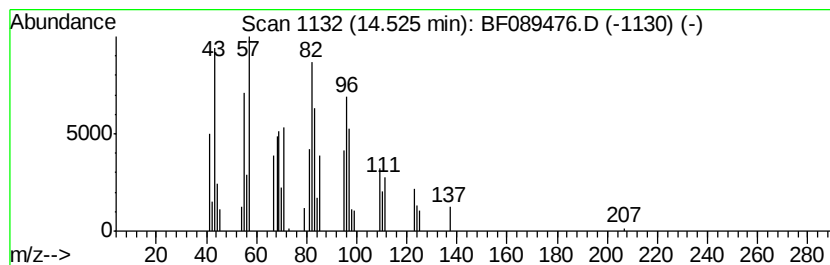
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Peak Number 7 Oxirane, hexadecyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.53	2.96 ng	32706	Perylene-d12	14.94

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Oxirane, hexadecyl-	268	C18H36O	007390-81-0	86
2		1,19-Eicosadiene	278	C20H38	014811-95-1	80
3		Pentadecanal-	226	C15H30O	002765-11-9	72
4		1,16-Hexadecanediol	258	C16H34O2	007735-42-4	64
5		Hexadecanal	240	C16H32O	000629-80-1	64



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.58	45.3	ng	523754	1	6.49	231099	20.0
2-Pentanone, 4-me...	5.47	2.4	ng	28158	1	6.49	231099	20.0
unknown6.26	6.26	113.3	ng	1308760	1	6.49	231099	20.0
Trichloroacetic a...	13.49	3.4	ng	39374	5	13.61	233976	20.0
Oxirane, hexadecyl-	14.53	3.0	ng	32706	6	14.94	221028	20.0