

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF061516\
Data File : BF088067.D
Acq On : 16 Jun 2016 7:22
Operator : UM/SJ
Sample : H3570-17
Misc :
ALS Vial : 38 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-19-COMP

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-BF060716.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	1.701	8	10	19	rVB	164508	339372	10.73%	1.459%
2	1.815	19	20	30	rVV	1733038	3162853	100.00%	13.595%
3	1.941	30	31	79	rVB	120402	697956	22.07%	3.000%
4	4.901	288	290	299	rBV	96006	136299	4.31%	0.586%
5	5.336	325	328	330	rBV	1725378	1976579	62.49%	8.496%
6	6.387	417	420	422	rBV	1716622	2051492	64.86%	8.818%
7	6.513	428	431	433	rBV	1746166	2059189	65.11%	8.851%
8	6.742	448	451	453	rBV	729099	607544	19.21%	2.611%
9	6.902	462	465	467	rBV	1526850	1663319	52.59%	7.149%
10	7.313	498	501	503	rBV	1212488	1362397	43.07%	5.856%
11	7.450	511	513	518	rBV	14857	34957	1.11%	0.150%
12	8.033	561	564	566	rBV	585851	768702	24.30%	3.304%
13	9.108	655	658	660	rBV	2384285	2128957	67.31%	9.151%
14	9.508	690	693	695	rBV	481640	505673	15.99%	2.173%
15	9.725	710	712	714	rBV	33597	33428	1.06%	0.144%
16	9.782	714	717	719	rVV	908382	847980	26.81%	3.645%
17	10.216	754	755	757	rVB	62150	58412	1.85%	0.251%
18	10.433	771	774	778	rBV	20990	43283	1.37%	0.186%
19	10.571	783	786	788	rBV	904115	1110449	35.11%	4.773%
20	10.696	795	797	801	rBV	57278	97018	3.07%	0.417%
21	11.142	834	836	837	rBV	32648	35745	1.13%	0.154%
22	11.256	844	846	849	rVB	752381	679301	21.48%	2.920%
23	12.845	982	985	987	rBV	1670921	1571354	49.68%	6.754%
24	13.748	1062	1064	1074	rBV	51331	108176	3.42%	0.465%
25	13.885	1074	1076	1079	rBV2	517912	586796	18.55%	2.522%
26	15.291	1196	1199	1202	rBV	464759	598192	18.91%	2.571%

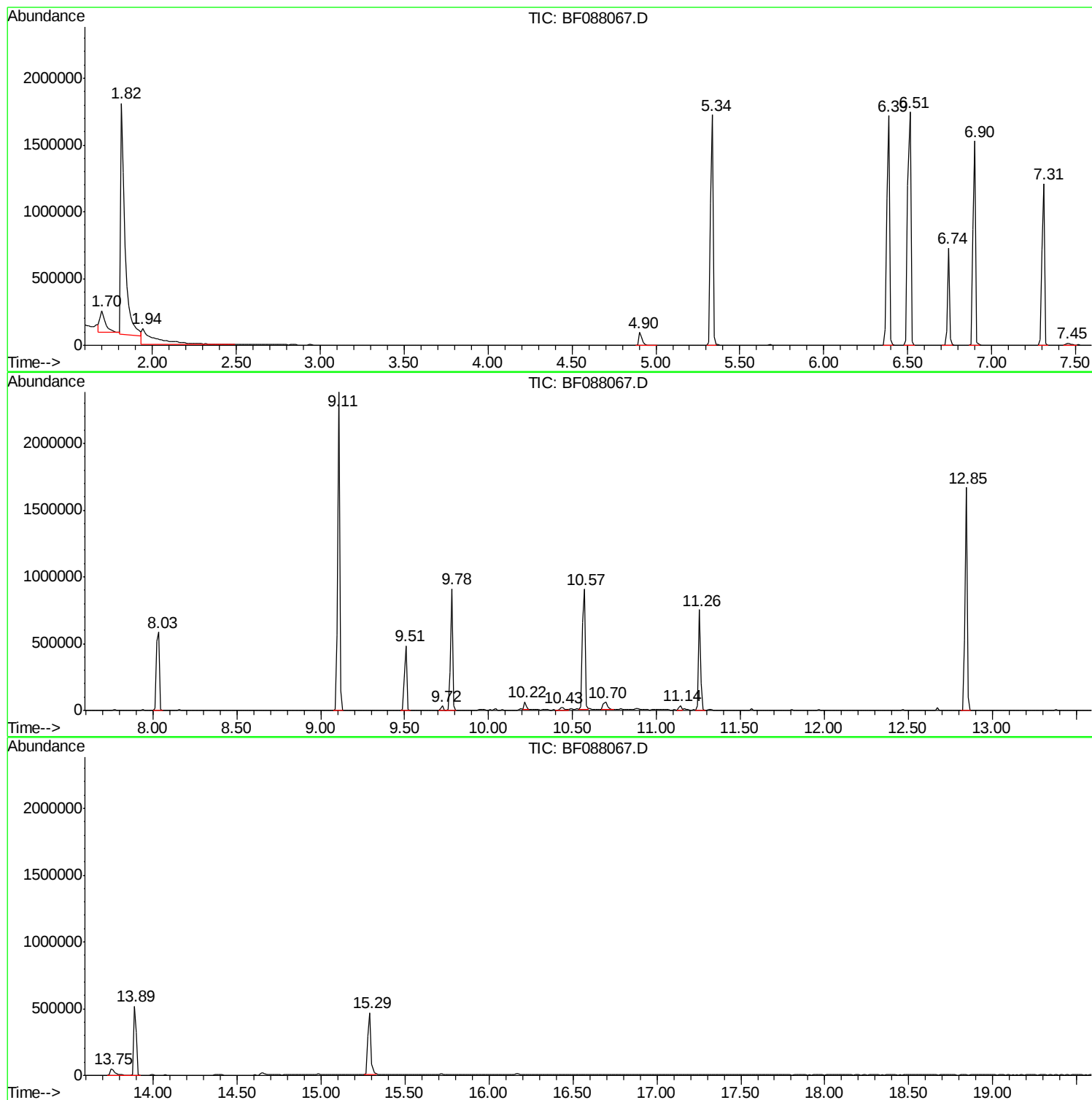
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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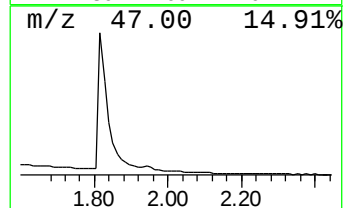
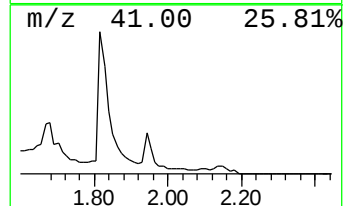
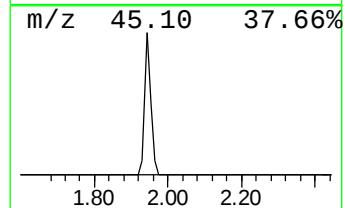
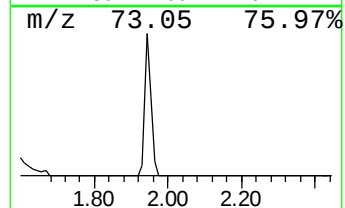
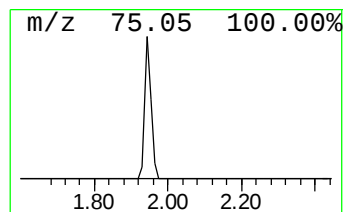
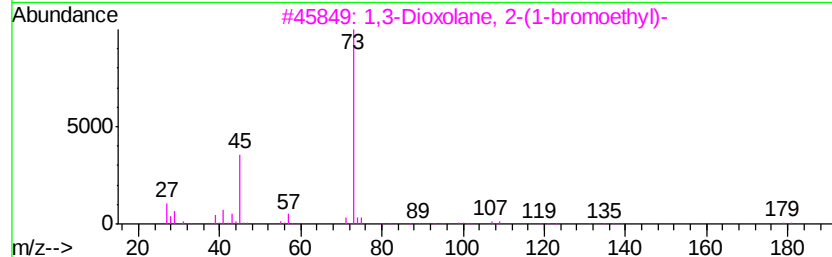
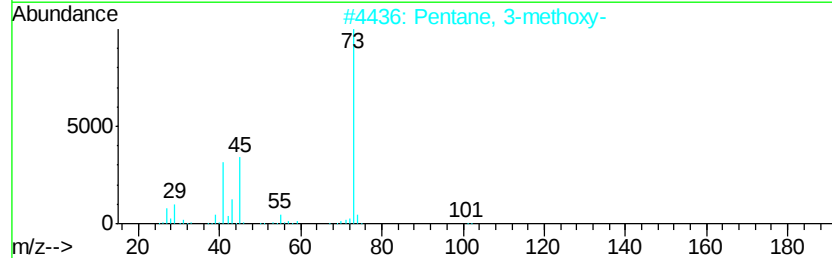
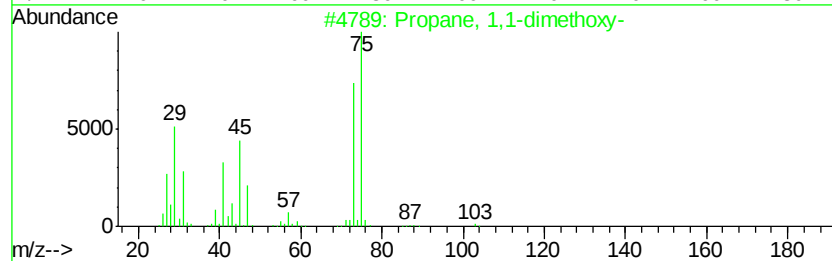
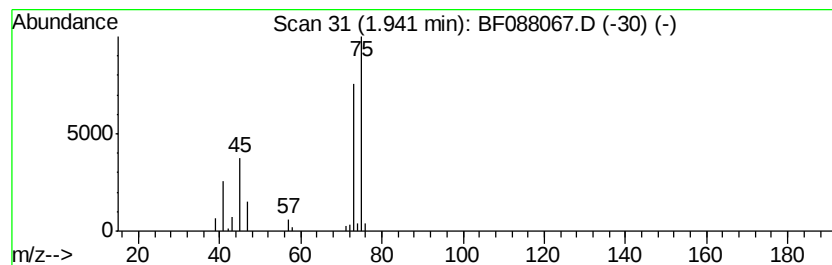
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Propane, 1,1-dimethoxy- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.94	22.98 ng	697956	1,4-Dichlorobenzene-d4	6.74

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	83
2		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	22
3		1,3-Dioxolane, 2-(1-bromoethyl)-	180	C5H9BrO2	005267-73-2	10
4		Glycine	75	C2H5NO2	000056-40-6	9
5		Thiocyanic acid, methyl ester	73	C2H3NS	000556-64-9	9



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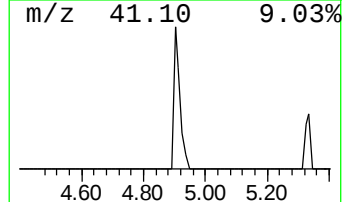
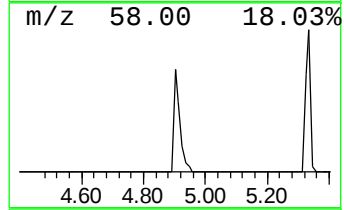
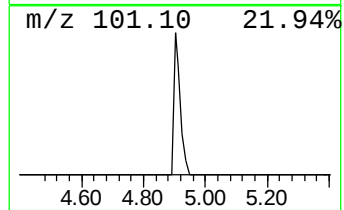
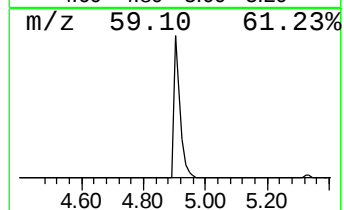
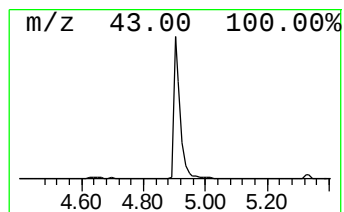
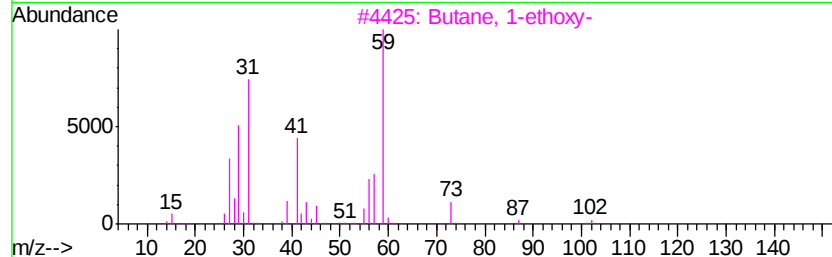
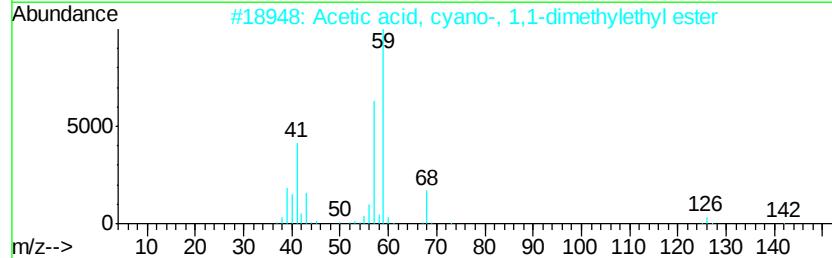
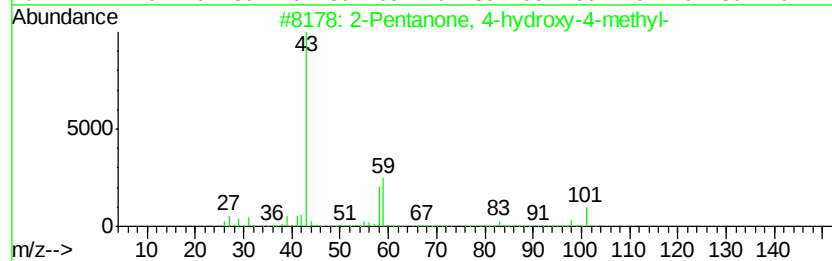
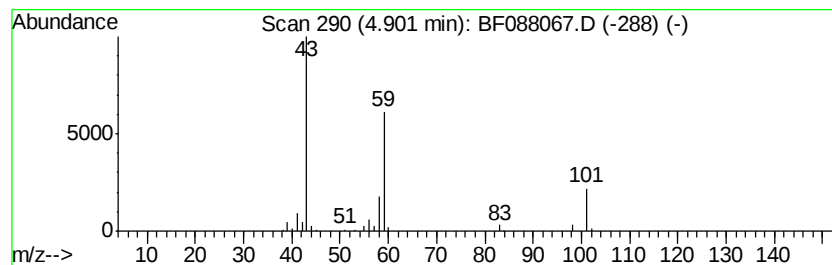
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.90	4.49 ng	136299	1,4-Dichlorobenzene-d4	6.74

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	23
3		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
4		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5		Acetone	58	C3H6O	000067-64-1	9



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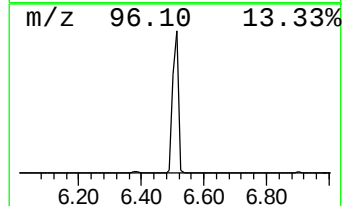
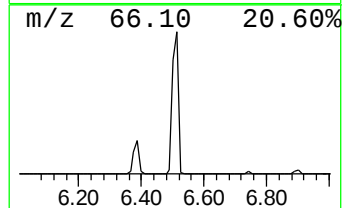
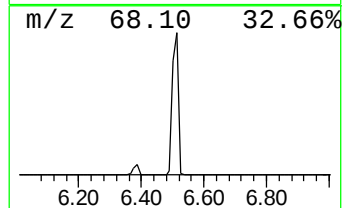
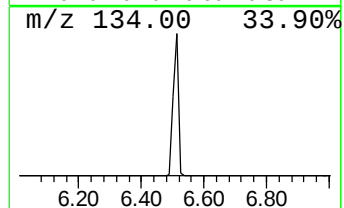
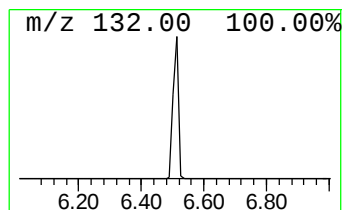
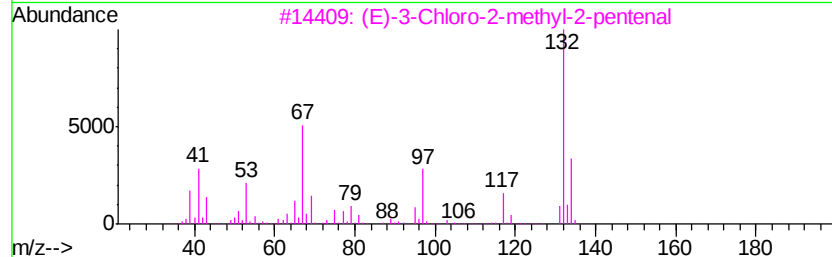
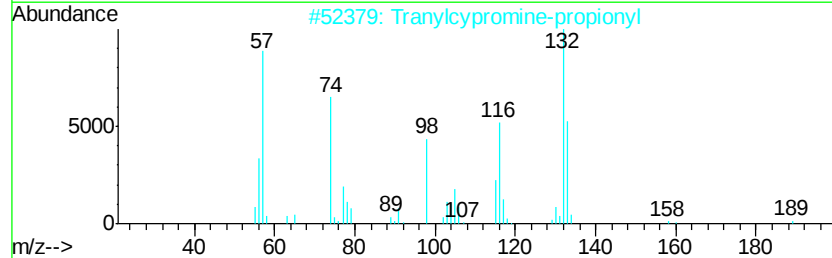
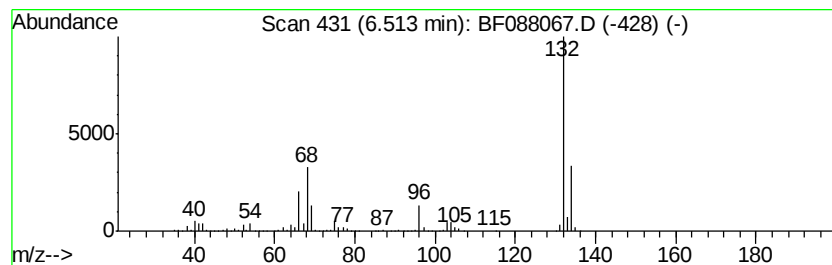
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Peak Number 5 unknown6.51 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.51	67.79 ng	2059190	1,4-Dichlorobenzene-d4	6.74

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
3		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
4		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9



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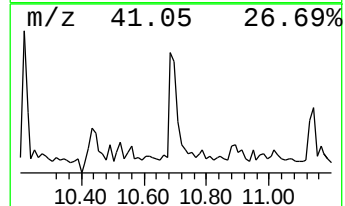
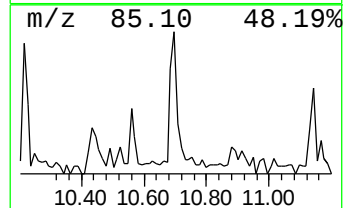
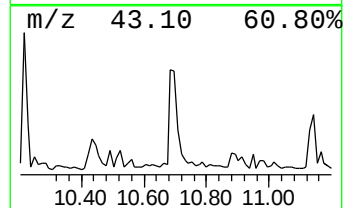
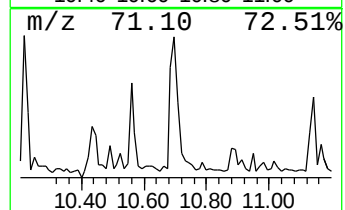
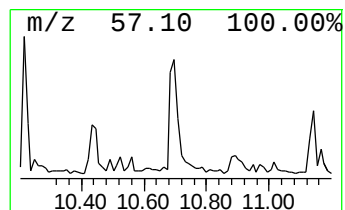
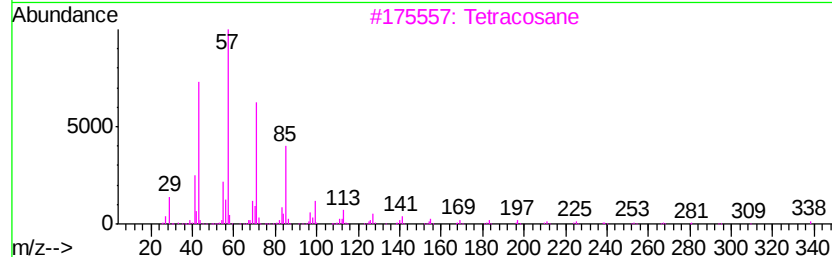
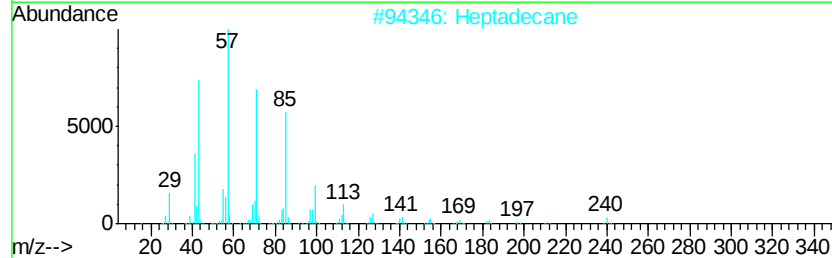
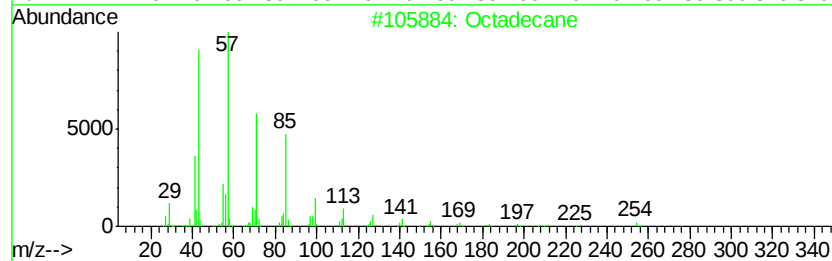
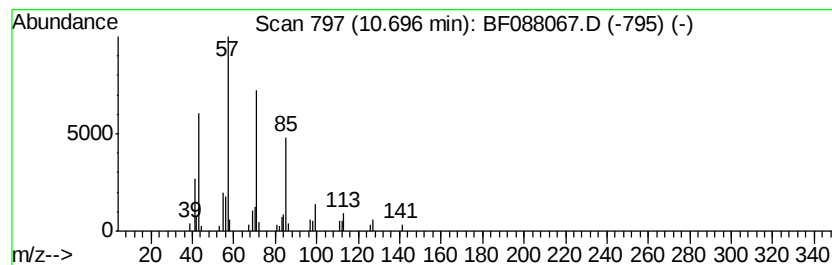
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Peak Number 7 Octadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.70	2.86 ng	97018	Phenanthrene-d10	11.26

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane		254	C18H38	000593-45-3	91
2	Heptadecane		240	C17H36	000629-78-7	91
3	Tetracosane		338	C24H50	000646-31-1	87
4	Hexadecane		226	C16H34	000544-76-3	87
5	Silane, trichlorooctadecyl-		386	C18H37Cl3Si	000112-04-9	86



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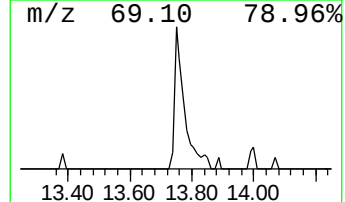
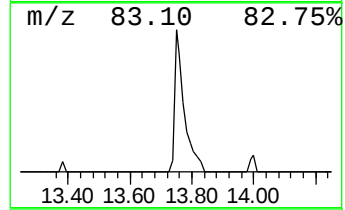
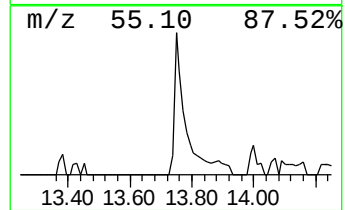
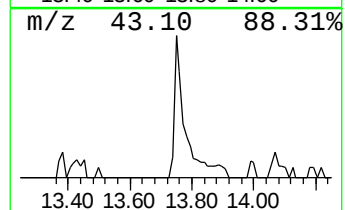
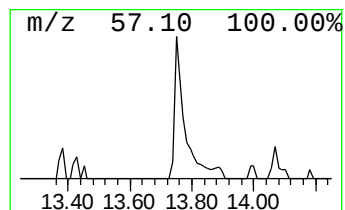
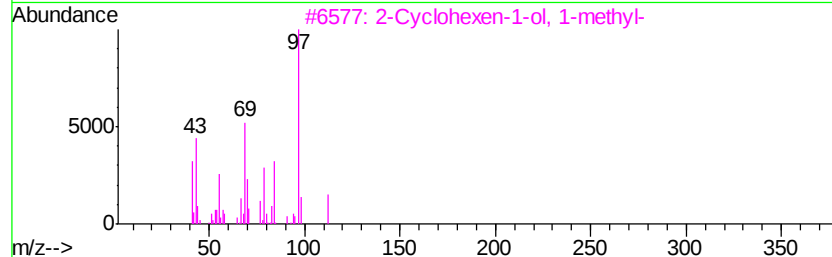
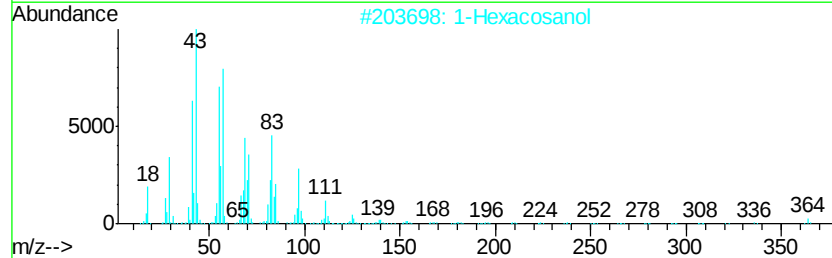
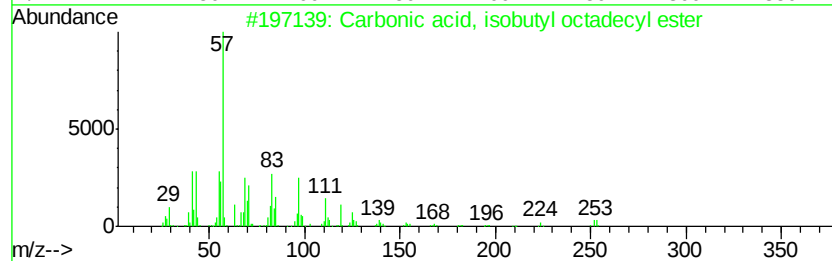
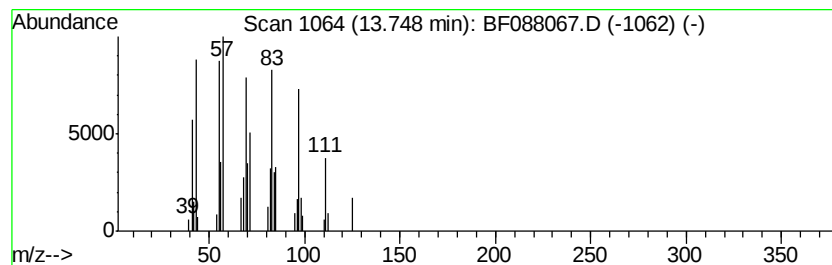
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Peak Number 8 Carbonic acid, isobutyl oct... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.75	3.69 ng	108176	Chrysene-d12	13.89

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Carbonic acid, isobutyl octadecyl...	370	C23H46O3	1000314-61-5	59
2		1-Hexacosanol	382	C26H54O	000506-52-5	52
3		2-Cyclohexen-1-ol, 1-methyl-	112	C7H12O	023758-27-2	43
4		Cycloheptane, methyl-	112	C8H16	004126-78-7	43
5		n-Tetracosanol-1	354	C24H50O	000506-51-4	38



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Propane, 1,1-dime...	1.94	23.0	ng	697956	1	6.74	607544	20.0
2-Pentanone, 4-hy...	4.90	4.5	ng	136299	1	6.74	607544	20.0
unknown6.51	6.51	67.8	ng	2059190	1	6.74	607544	20.0
Octadecane	10.70	2.9	ng	97018	4	11.26	679301	20.0
Carbonic acid, is...	13.75	3.7	ng	108176	5	13.89	586796	20.0