

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF083116\
Data File : BF089956.D
Acq On : 31 Aug 2016 17:56
Operator : UM/SJ
Sample : H4645-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MSP-BPM

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-BF083116.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	1.644	3	5	12	rVB	30643	71723	1.37%	0.163%
2	1.747	12	14	32	rVB	388804	892956	17.02%	2.026%
3	4.764	276	278	286	rVB	717628	1222074	23.30%	2.773%
4	5.210	314	317	320	rBV	3116568	4729022	90.16%	10.730%
5	6.285	407	411	413	rBV	3447157	5067185	96.61%	11.497%
6	6.399	418	421	424	rBV	4035200	4271722	81.44%	9.692%
7	6.639	439	442	444	rBV	997816	1106925	21.10%	2.512%
8	6.787	453	455	458	rBV	2847309	3460469	65.97%	7.851%
9	7.199	488	491	494	rBV	2366116	2761651	52.65%	6.266%
10	7.919	552	554	556	rBV	1805114	1471958	28.06%	3.340%
11	9.005	646	649	651	rBV	3719570	5245147	100.00%	11.901%
12	9.393	681	683	685	rBV	1289969	1030601	19.65%	2.338%
13	9.668	704	707	709	rBV	1434467	1565402	29.84%	3.552%
14	10.113	745	746	748	rVB	109374	94619	1.80%	0.215%
15	10.331	762	765	769	rBV	43839	85746	1.63%	0.195%
16	10.445	772	775	778	rVV	2740528	2654319	50.61%	6.022%
17	10.582	786	787	794	rVB	146765	214359	4.09%	0.486%
18	11.028	824	826	828	rBV	69095	73062	1.39%	0.166%
19	11.131	833	835	838	rVB	1540134	1368501	26.09%	3.105%
20	12.719	971	974	976	rBV	4000913	3948444	75.28%	8.959%
21	13.634	1051	1054	1061	rBV2	159782	252809	4.82%	0.574%
22	13.748	1061	1064	1066	rBV	1278802	1196663	22.81%	2.715%
23	14.605	1137	1139	1142	rBV	127463	158833	3.03%	0.360%
24	15.097	1179	1182	1184	rBV	933274	1129859	21.54%	2.564%

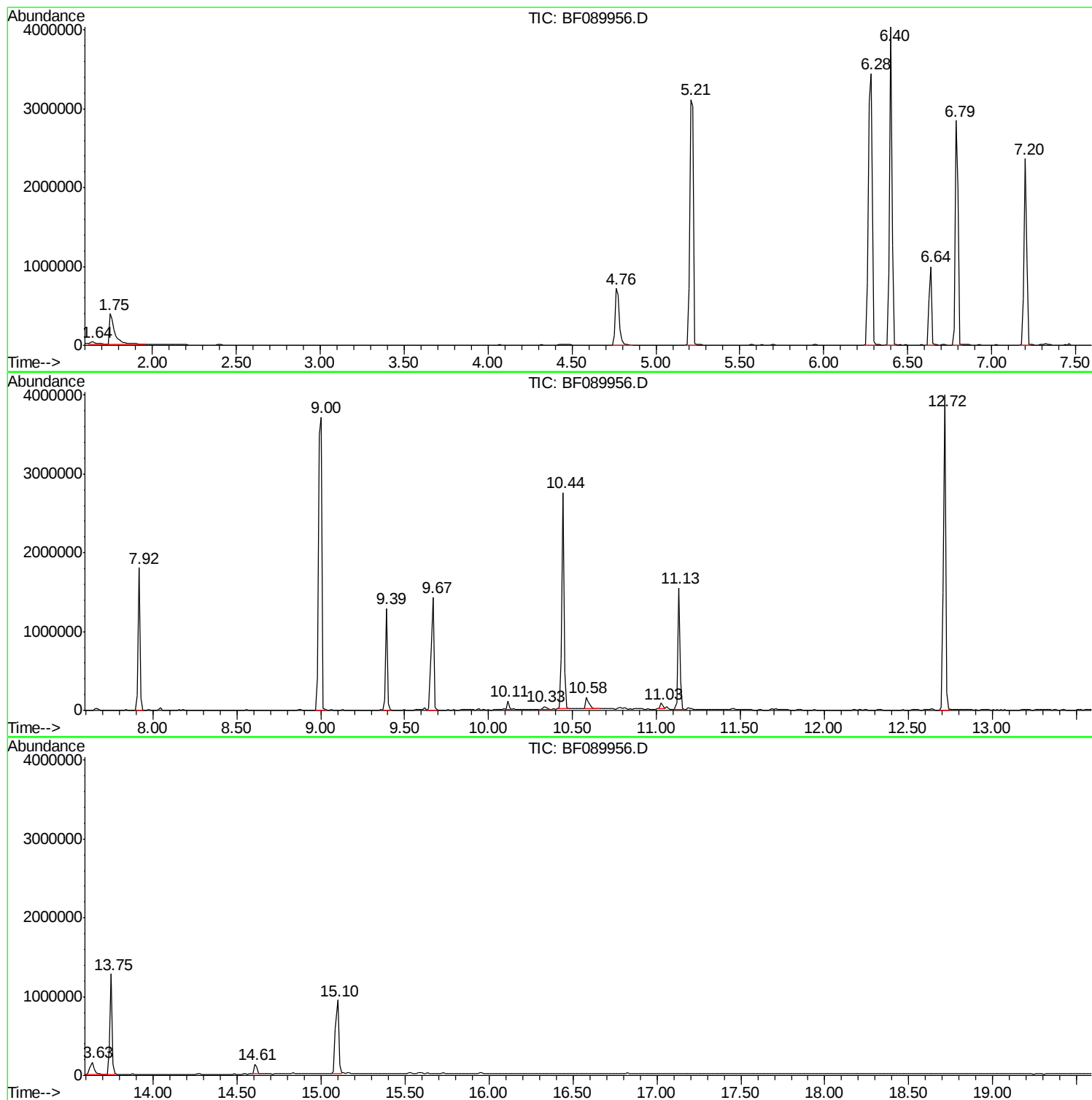
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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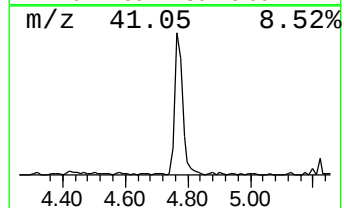
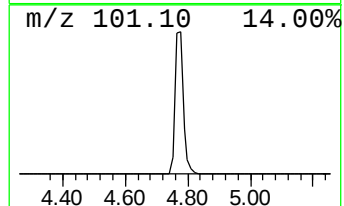
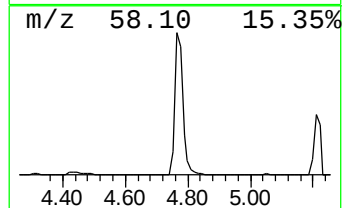
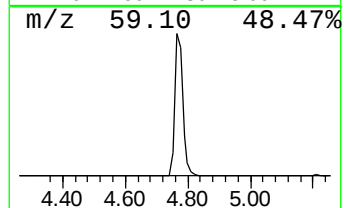
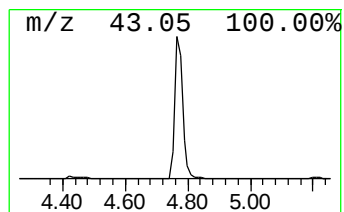
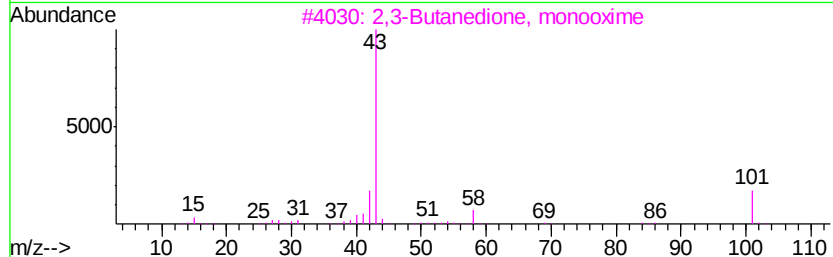
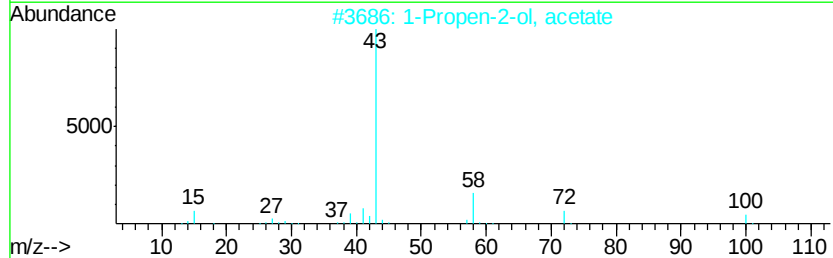
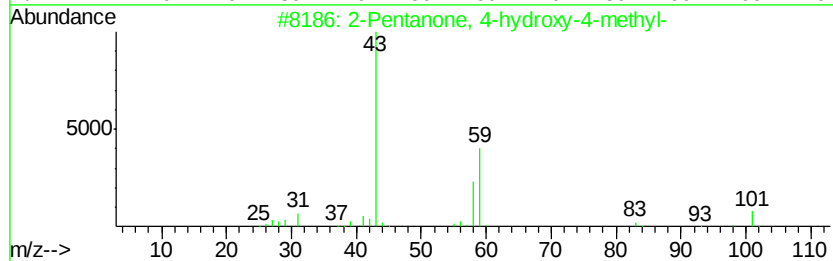
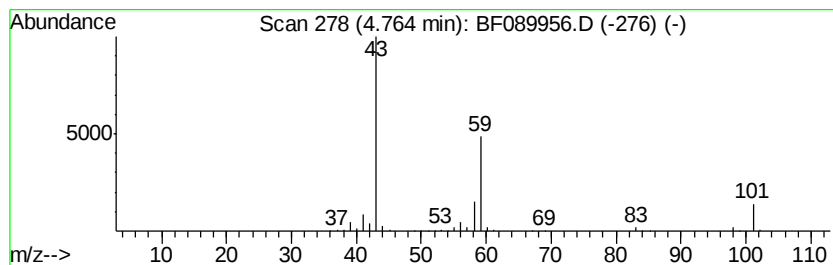
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF083116.M
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.76	22.08 ng	1222070	1,4-Dichlorobenzene-d4	6.64

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
3		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	9
5		Formamide, N,N-diethyl-	101	C5H11NO	000617-84-5	7



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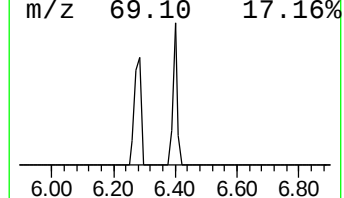
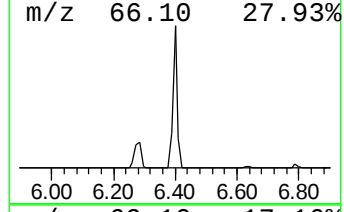
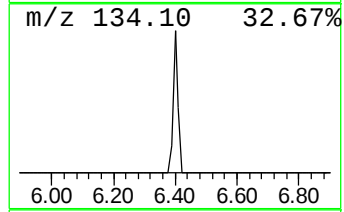
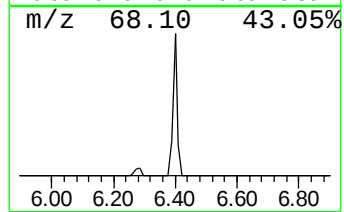
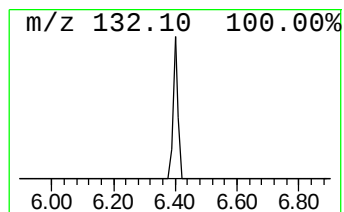
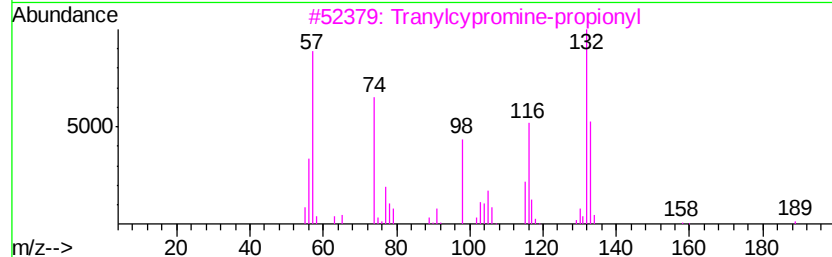
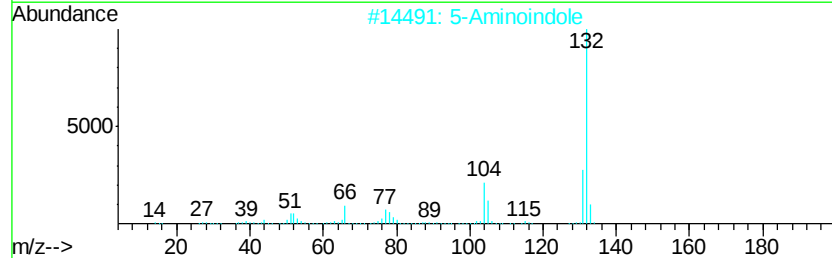
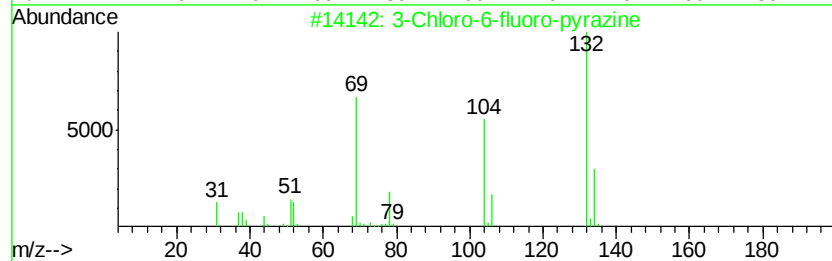
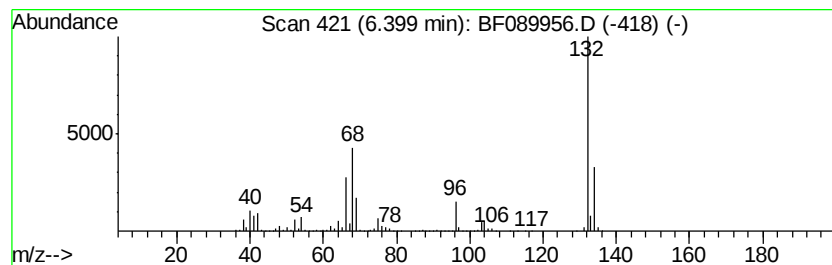
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Peak Number 3 unknown6.40 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.40	77.18 ng	4271720	1,4-Dichlorobenzene-d4	6.64

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Aminoindole	132	C8H8N2	005192-03-0	12
3		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5		Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9



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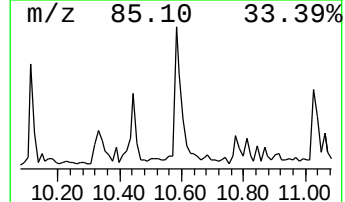
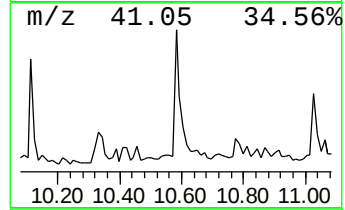
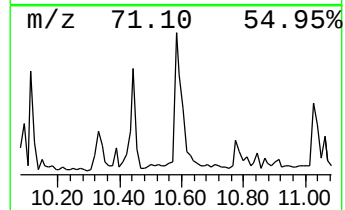
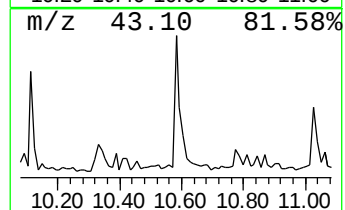
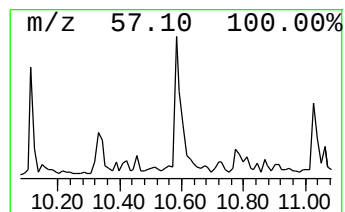
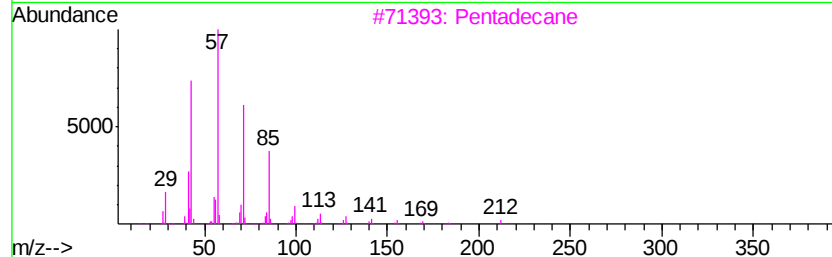
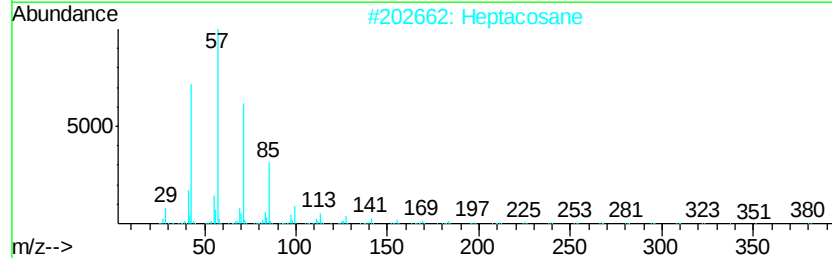
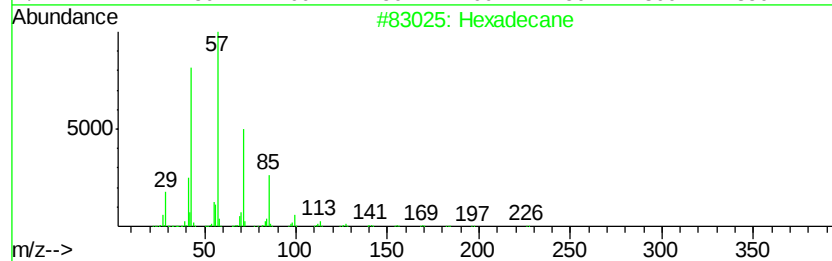
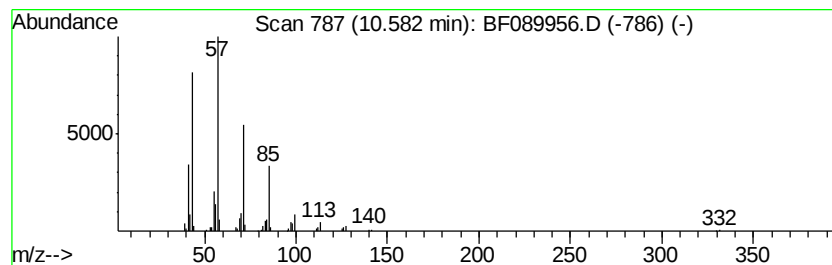
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Peak Number 5 Hexadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.58	3.13 ng	214359	Phenanthrene-d10	11.13

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane		226	C16H34	000544-76-3	91
2	Heptacosane		380	C27H56	000593-49-7	90
3	Pentadecane		212	C15H32	000629-62-9	90
4	Heptadecane		240	C17H36	000629-78-7	90
5	Tridecane		184	C13H28	000629-50-5	86



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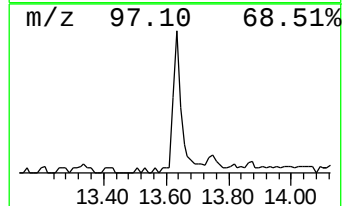
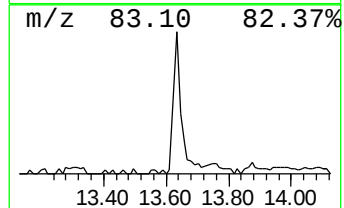
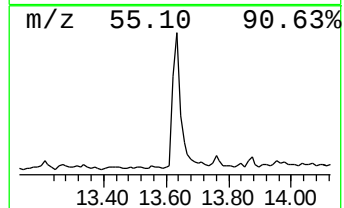
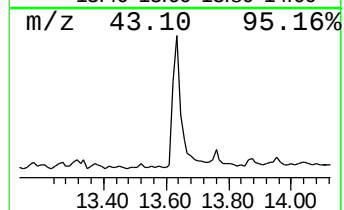
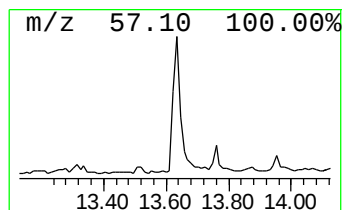
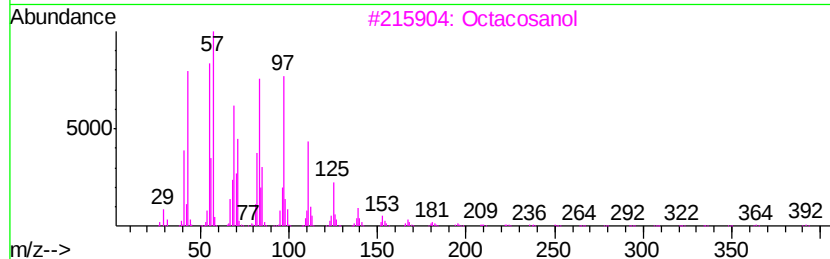
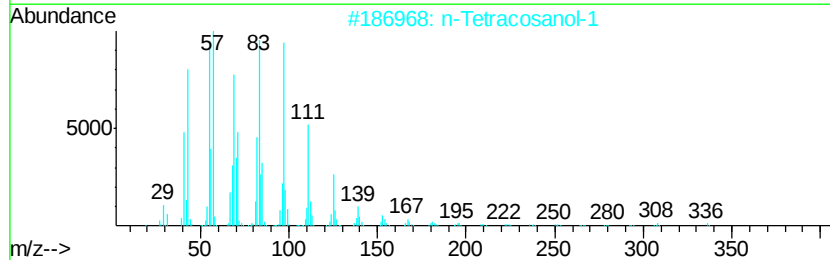
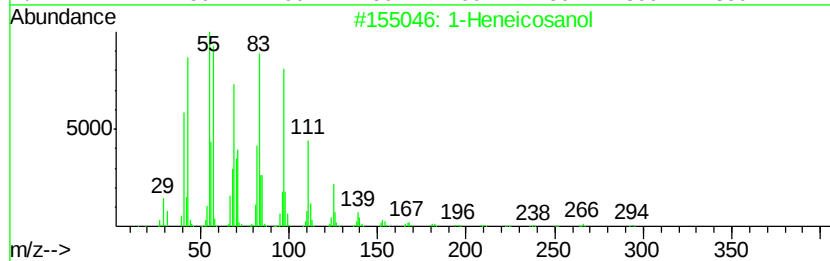
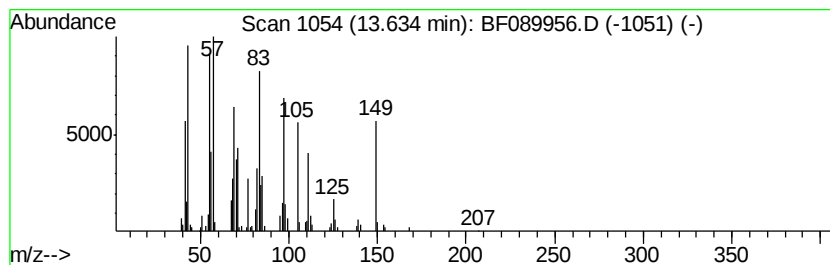
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Peak Number 6 1-Heneicosanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.63	4.23 ng	252809	Chrysene-d12	13.75

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Heneicosanol	312	C21H44O	015594-90-8	93
2		n-Tetracosanol-1	354	C24H50O	000506-51-4	93
3		Octacosanol	410	C28H58O	000557-61-9	91
4		1-Heptacosanol	396	C27H56O	002004-39-9	87
5		1-Nonadecene	266	C19H38	018435-45-5	87



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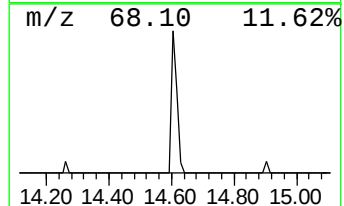
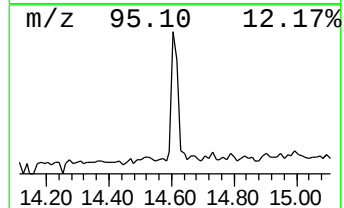
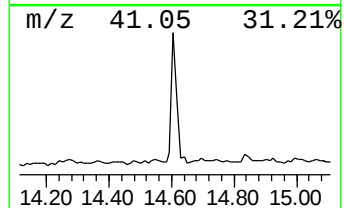
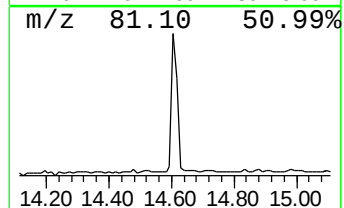
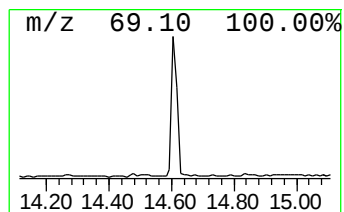
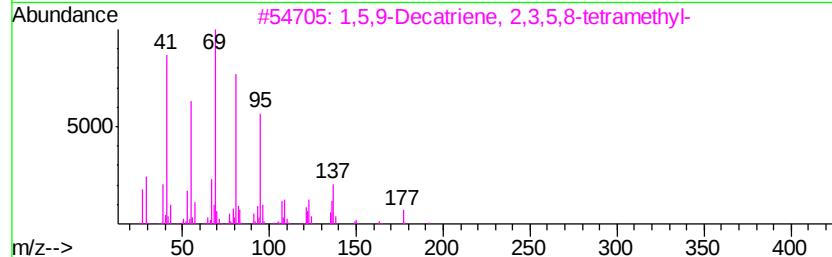
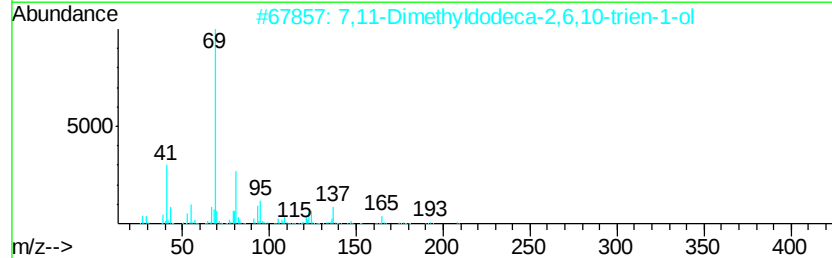
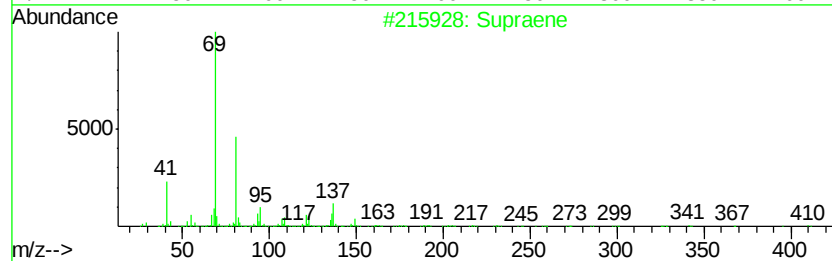
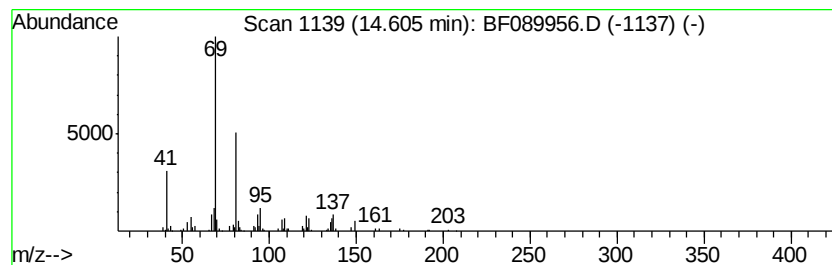
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Peak Number 7 Supraene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.61	2.81 ng	158833	Perylene-d12	15.10

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Supraene	410	C30H50	007683-64-9	91
2		7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	72
3		1,5,9-Decatriene, 2,3,5,8-tetram...	192	C14H24	230646-72-7	64
4		2,3,5-Trimethyl-2,3,5-hexanetric...	203	C12H17N3	003974-79-6	59
5		1,5-Heptadiene, 3,3,6-trimethyl-	138	C10H18	035387-63-4	58



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.76	22.1	ng	1222070	1	6.64	1106930	20.0
unknown6.40	6.40	77.2	ng	4271720	1	6.64	1106930	20.0
Hexadecane	10.58	3.1	ng	214359	4	11.13	1368500	20.0
1-Heneicosanol	13.63	4.2	ng	252809	5	13.75	1196660	20.0
Supraene	14.61	2.8	ng	158833	6	15.10	1129860	20.0