

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF101218\
 Data File : BF109868.D
 Acq On : 13 Oct 2018 7:20
 Operator : JU/SJ
 Sample : J5444-11
 Misc :
 ALS Vial : 42 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 101018-TIPC-F-D-B

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:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100818.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	4.881	472	475	489	rBV	65220	97323	2.71%	0.531%
2	5.310	545	548	576	rBV	477643	761364	21.22%	4.155%
3	6.339	720	723	740	rBV	278171	535623	14.93%	2.923%
4	6.463	741	744	770	rVV	1590234	1727523	48.15%	9.427%
5	6.692	780	783	805	rBV	414051	589723	16.44%	3.218%
6	6.851	805	810	831	rBV	2445633	2502635	69.76%	13.657%
7	7.263	875	880	906	rBV	1578069	2071192	57.73%	11.302%
8	7.975	997	1001	1029	rBV	523230	721395	20.11%	3.937%
9	9.051	1179	1184	1202	rBV	3362818	3587498	100.00%	19.577%
10	9.445	1248	1251	1260	rBV	40251	47904	1.34%	0.261%
11	9.722	1294	1298	1317	rVB	685992	704949	19.65%	3.847%
12	10.398	1410	1413	1417	rBV	47062	36395	1.01%	0.199%
13	10.504	1428	1431	1450	rBV	762269	1060427	29.56%	5.787%
14	11.198	1546	1549	1573	rBV	366676	541991	15.11%	2.958%
15	12.780	1814	1818	1836	rBV	2254371	2262872	63.08%	12.348%
16	13.827	1992	1996	2012	rBV	390088	502528	14.01%	2.742%
17	14.657	2133	2137	2140	rBV	60756	57237	1.60%	0.312%
18	14.898	2174	2178	2184	rBV	38676	45987	1.28%	0.251%
19	15.227	2229	2234	2246	rBV	210237	412528	11.50%	2.251%
20	15.645	2299	2305	2312	rBV	34294	58241	1.62%	0.318%

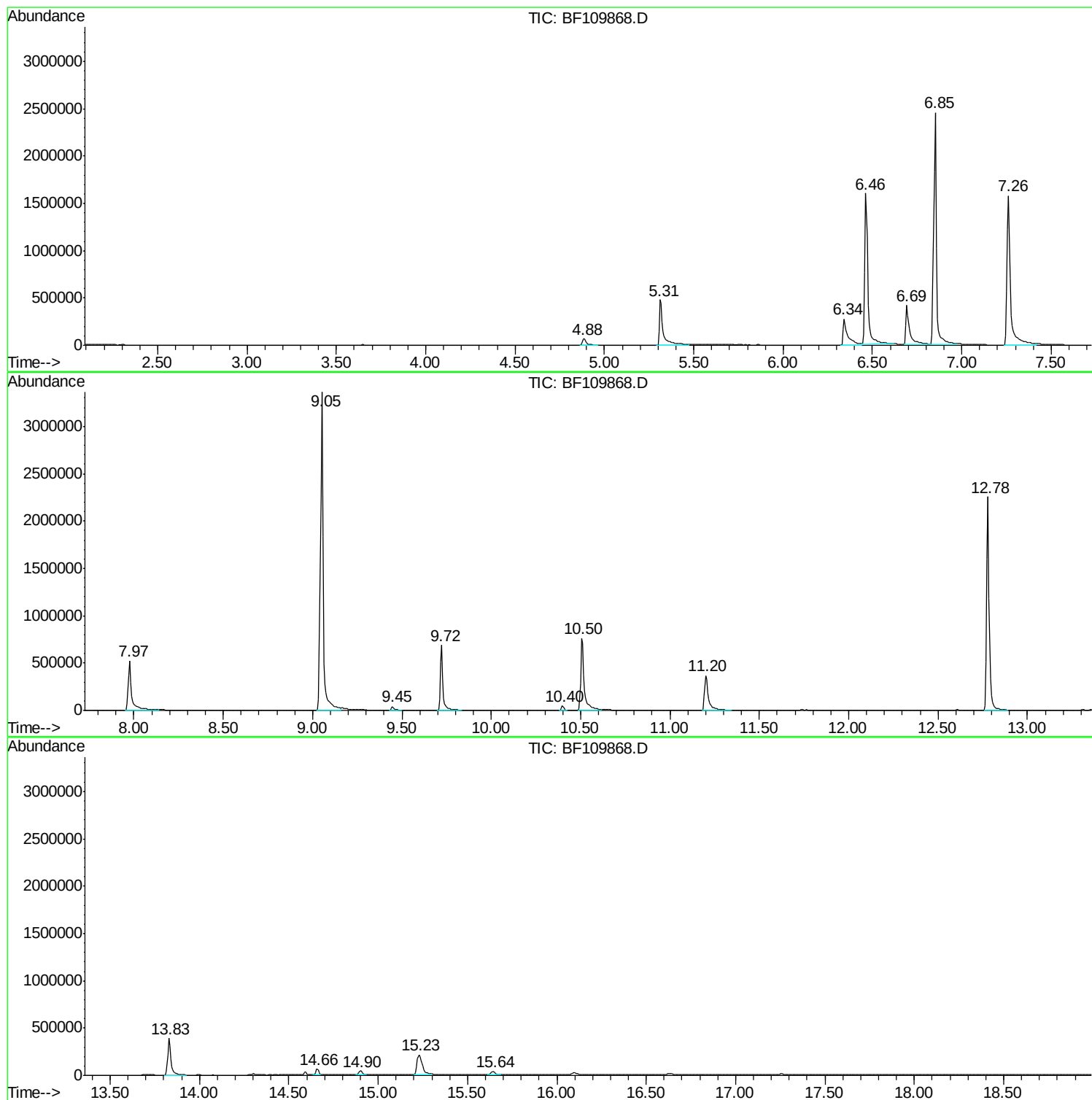
Sum of corrected areas: 18325335

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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF100818.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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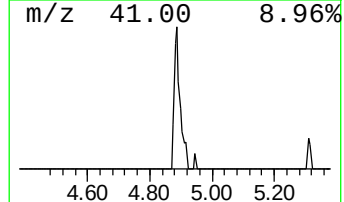
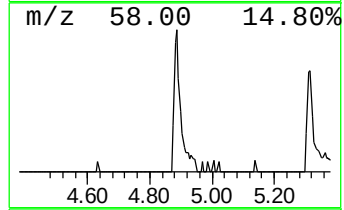
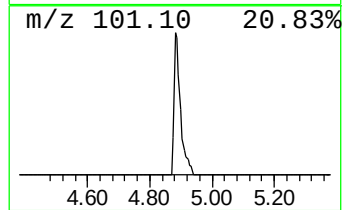
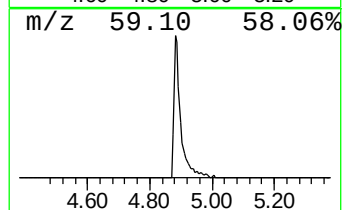
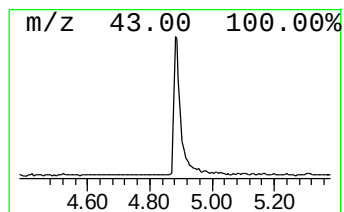
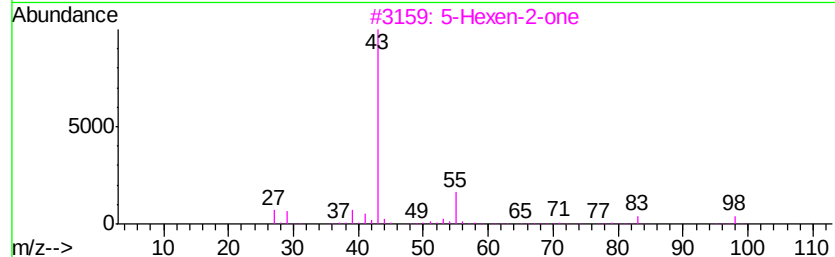
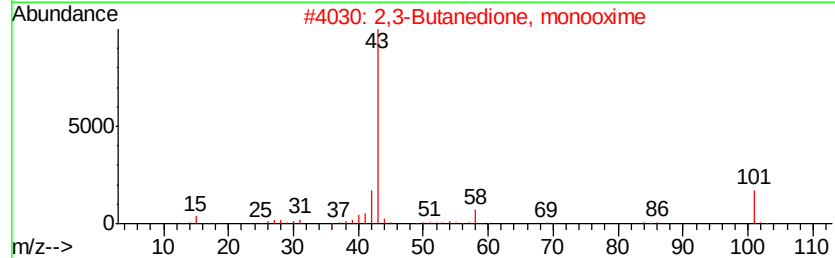
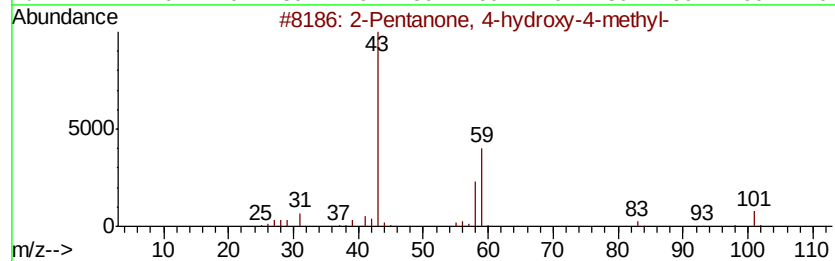
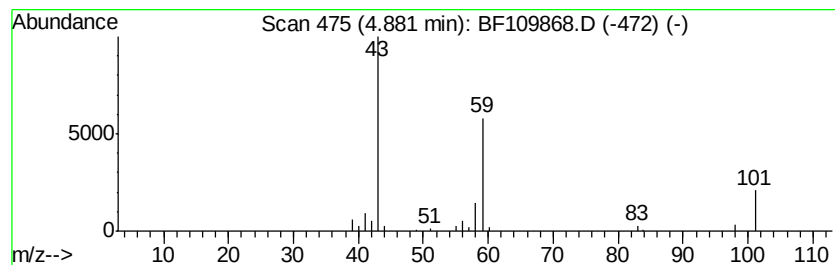
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.88	3.30 ng	97323	1,4-Dichlorobenzene-d4	6.69

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	40
2			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
3			5-Hexen-2-one	98	C6H10O	000109-49-9	9
4			2-Propanone, 1-(1-methylethoxy)-	116	C6H12O2	042781-12-4	9
5			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	9



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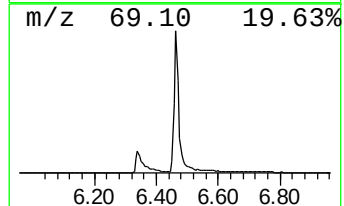
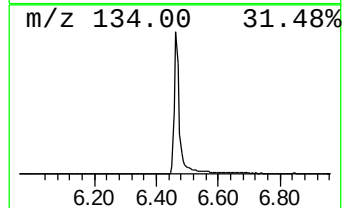
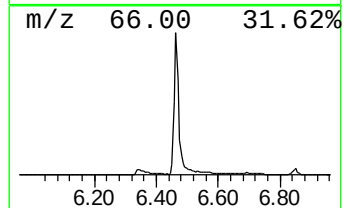
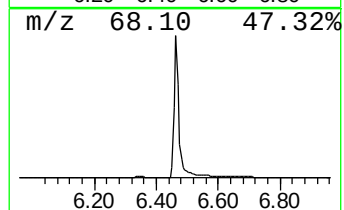
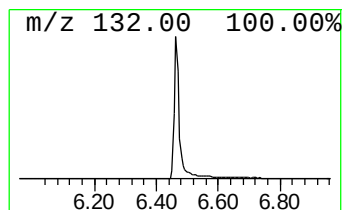
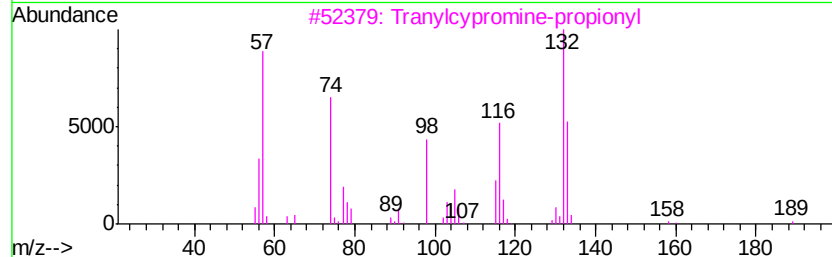
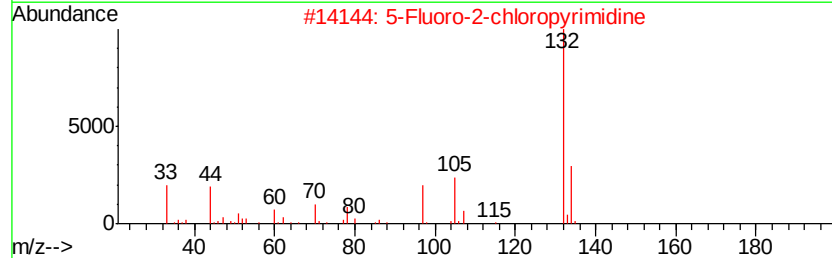
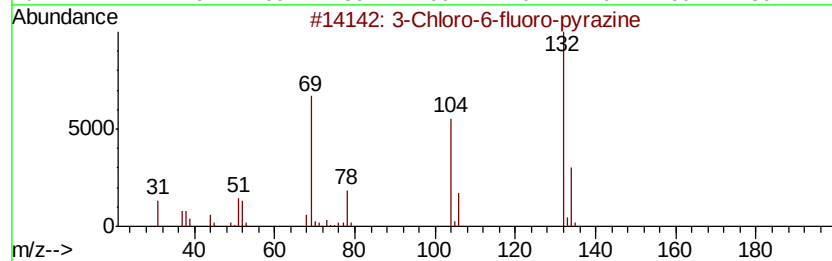
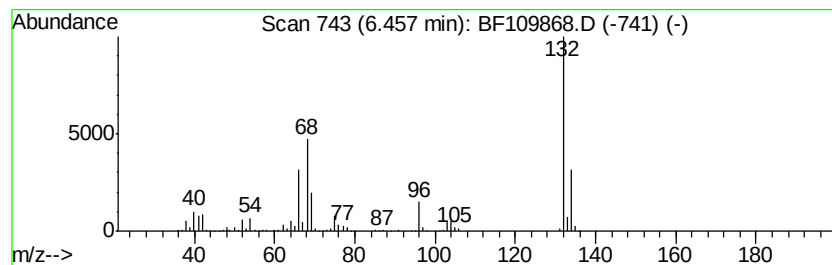
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Peak Number 2 unknown6.46 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.46	58.59 ng	1727520	1,4-Dichlorobenzene-d4	6.69

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
3		Tranvlcyproline-propionyl	189	C12H15NO	1000123-86-3	10
4		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5		1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	9



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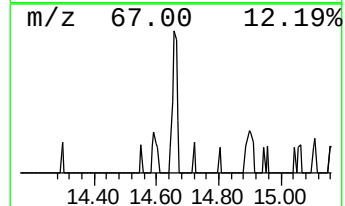
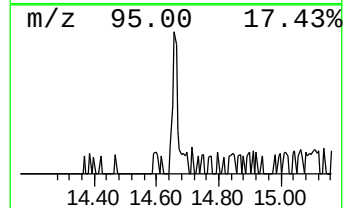
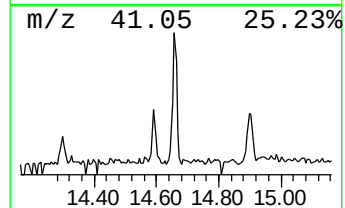
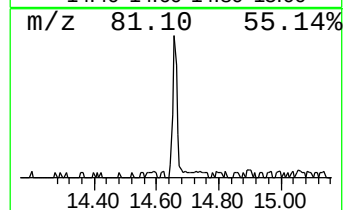
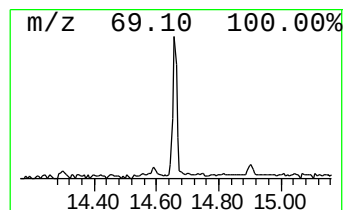
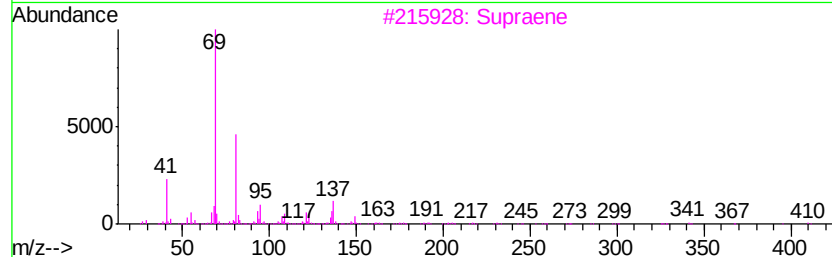
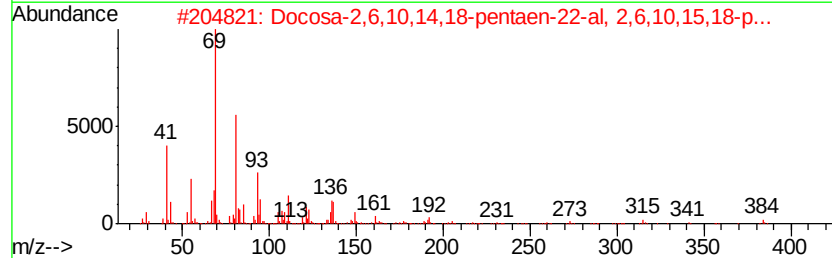
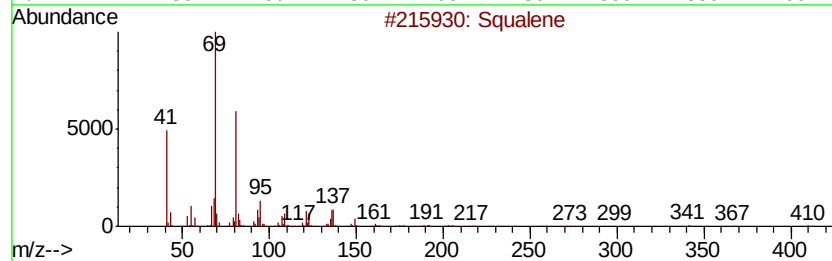
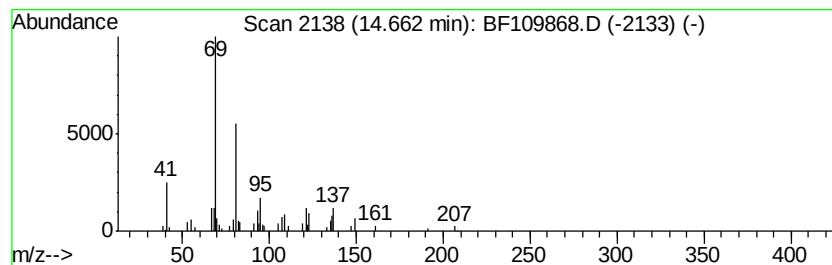
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Peak Number 4 Squalene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.66	2.77 ng	57237	Perylene-d12	15.23

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Squalene	410	C30H50	000111-02-4	91
2		Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	90
3		Supraene	410	C30H50	007683-64-9	87
4		Hexadeca-2,6,10,14-tetraen-1-ol,...	290	C20H34O	007614-21-3	83
5		2,6,10,14,18-Pentamethyl-2,6,10,...	342	C25H42	075581-03-2	83



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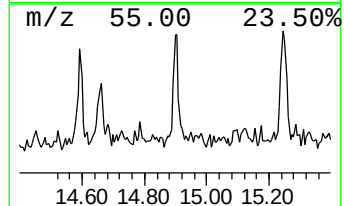
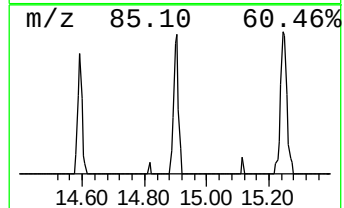
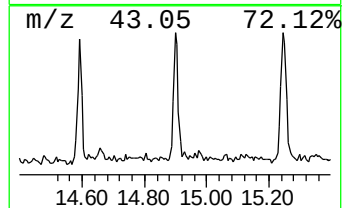
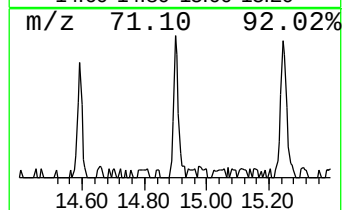
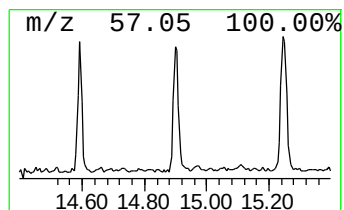
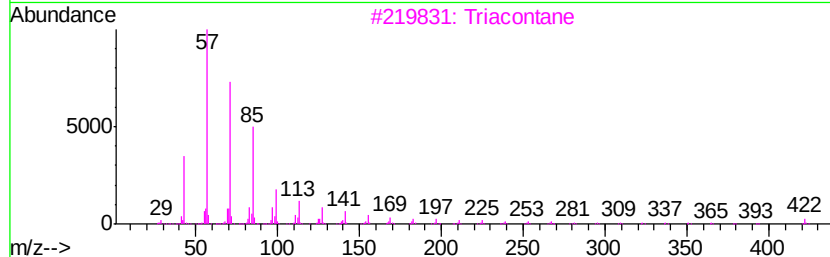
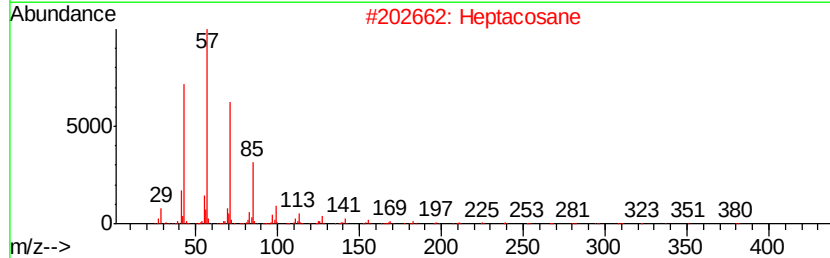
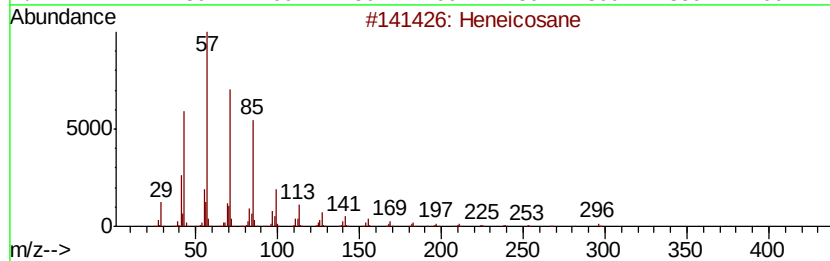
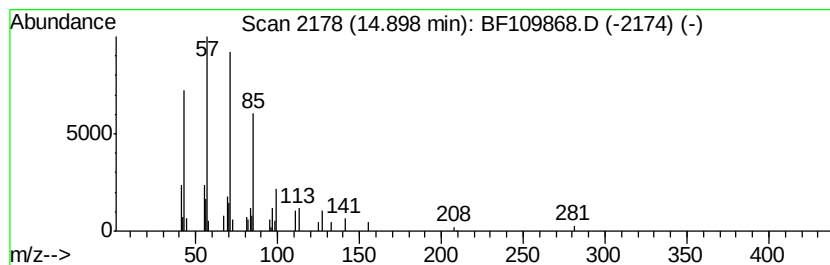
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Peak Number 5 Heneicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.90	2.23 ng	45987	Perylene-d12	15.23

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane		296	C21H44	000629-94-7	91
2	Heptacosane		380	C27H56	000593-49-7	90
3	Triacontane		422	C30H62	000638-68-6	90
4	Hexacosane		366	C26H54	000630-01-3	87
5	2-Bromotetradecane		276	C14H29Br	074036-95-6	86



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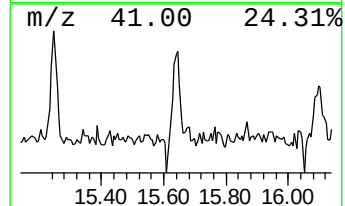
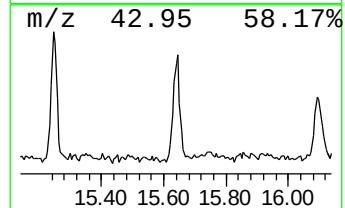
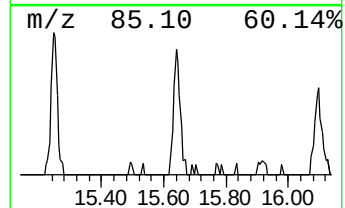
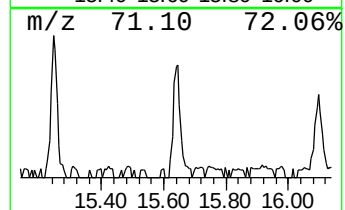
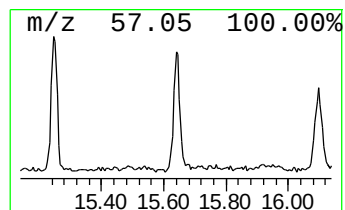
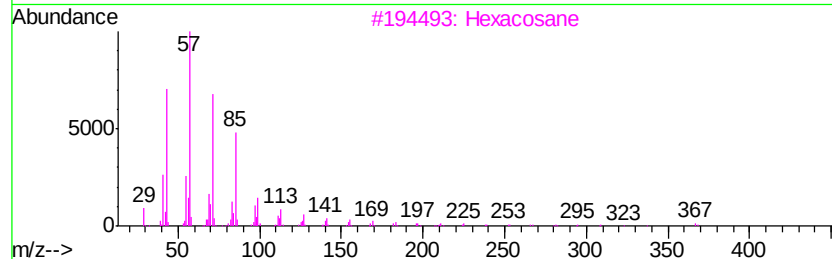
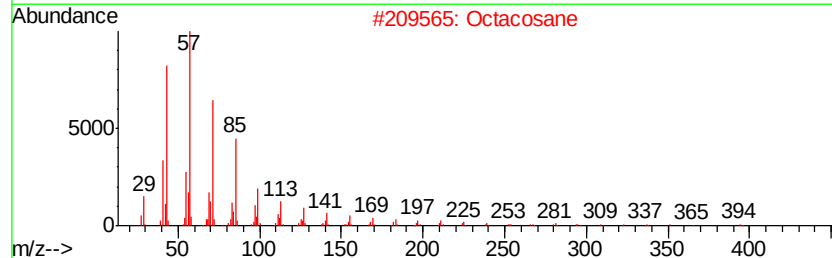
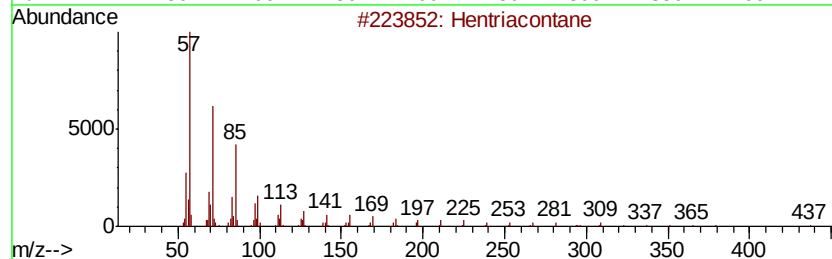
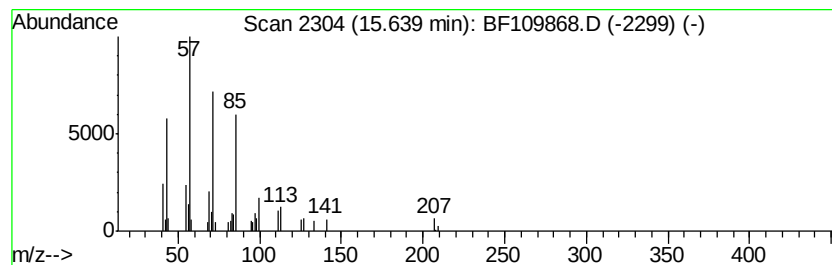
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Peak Number 6 Hentriacontane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.64	2.82 ng	58241	Perylene-d12	15.23

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hentriacontane	437	C31H64	000630-04-6	91
2		Octacosane	394	C28H58	000630-02-4	91
3		Hexacosane	366	C26H54	000630-01-3	87
4		Heneicosane	296	C21H44	000629-94-7	87
5		Heptacosane	380	C27H56	000593-49-7	87



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.88	3.3	ng	97323	1	6.69	589723	20.0
unknown6.46	6.46	58.6	ng	1727520	1	6.69	589723	20.0
Squalene	14.66	2.8	ng	57237	6	15.23	412528	20.0
Heneicosane	14.90	2.2	ng	45987	6	15.23	412528	20.0
Hentriacontane	15.64	2.8	ng	58241	6	15.23	412528	20.0