

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF101617\
 Data File : BF099558.D
 Acq On : 16 Oct 2017 21:50
 Operator : SJ/JU
 Sample : I5782-06
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 S3(10-12)

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-BF092317.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	5.075	504	508	522	rBV	338258	469443	17.21%	2.129%
2	5.475	571	576	599	rBV	2126237	2322498	85.12%	10.532%
3	6.481	742	747	766	rBV	2078200	2460435	90.18%	11.158%
4	6.616	766	770	773	rBV	2594542	2369000	86.83%	10.743%
5	6.845	805	809	816	rBV	658891	589204	21.60%	2.672%
6	6.998	831	835	839	rBV	2080962	1868075	68.47%	8.471%
7	7.410	900	905	908	rBV	1534182	1459135	53.48%	6.617%
8	8.122	1023	1026	1035	rBV	876273	814196	29.84%	3.692%
9	8.681	1118	1121	1126	rBV	37731	31216	1.14%	0.142%
10	9.198	1204	1209	1212	rBV	2803985	2728381	100.00%	12.373%
11	9.592	1273	1276	1288	rVB	671345	528224	19.36%	2.395%
12	9.881	1321	1325	1329	rBV2	1042917	878619	32.20%	3.984%
13	10.592	1443	1446	1453	rVB	101218	78367	2.87%	0.355%
14	10.675	1456	1460	1463	rBV	1449762	1320895	48.41%	5.990%
15	11.369	1574	1578	1582	rBV	930637	792047	29.03%	3.592%
16	12.951	1843	1847	1851	rBV	2111573	2028817	74.36%	9.200%
17	13.833	1993	1997	2010	rBV2	87111	124390	4.56%	0.564%
18	14.010	2024	2027	2035	rBV	540596	535512	19.63%	2.428%
19	14.833	2164	2167	2171	rVB	111997	103660	3.80%	0.470%
20	15.486	2272	2278	2287	rVB	430031	549233	20.13%	2.491%

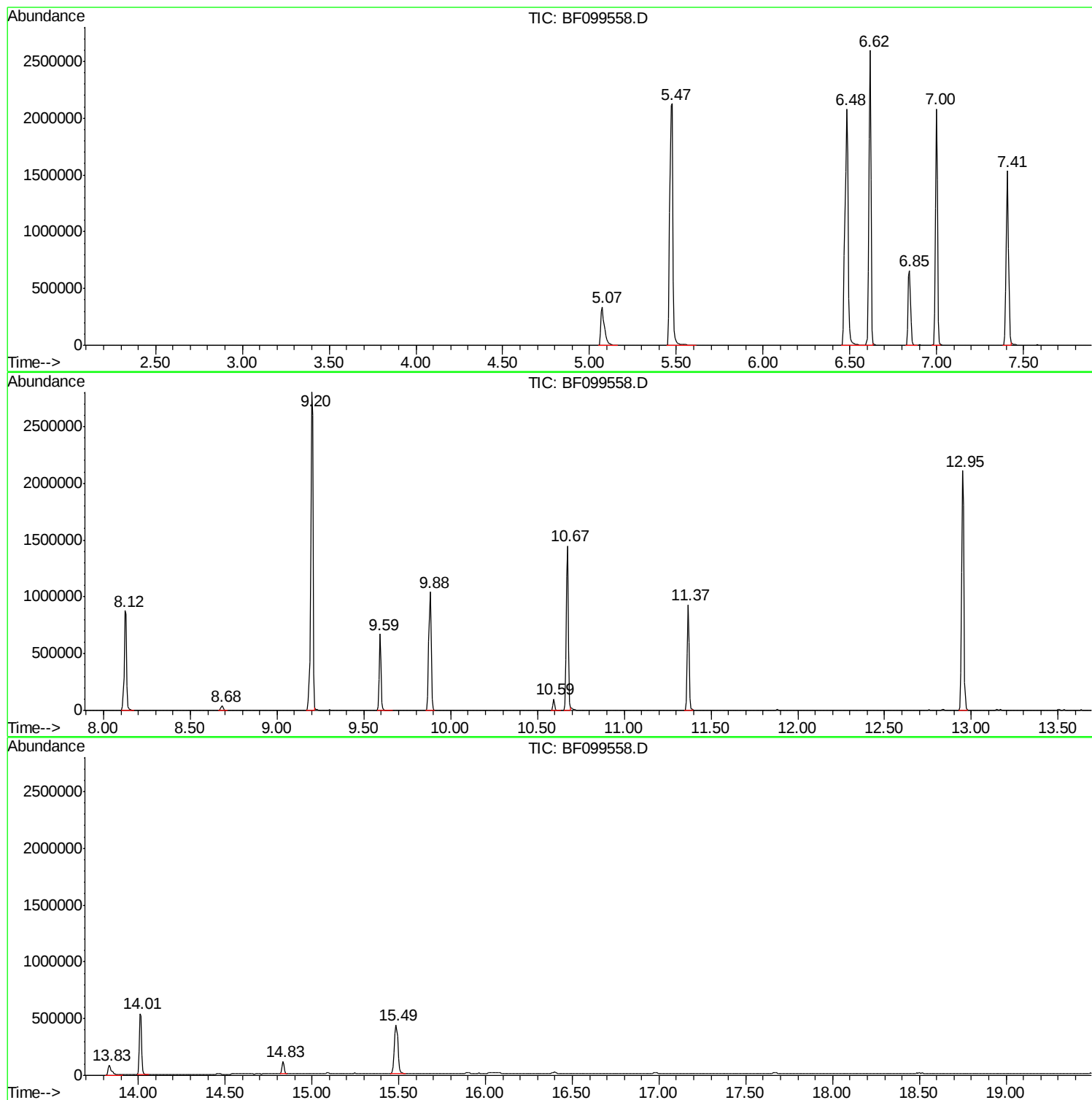
Sum of corrected areas: 22051347

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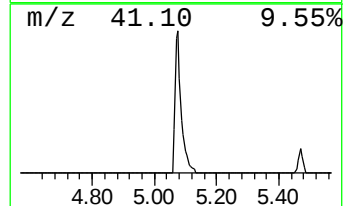
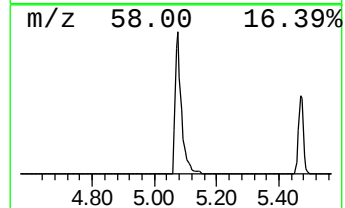
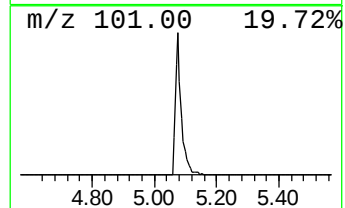
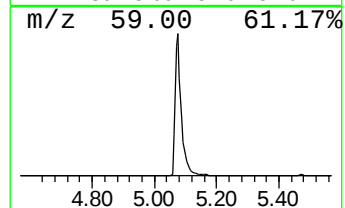
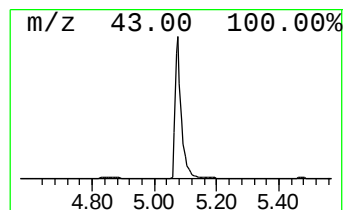
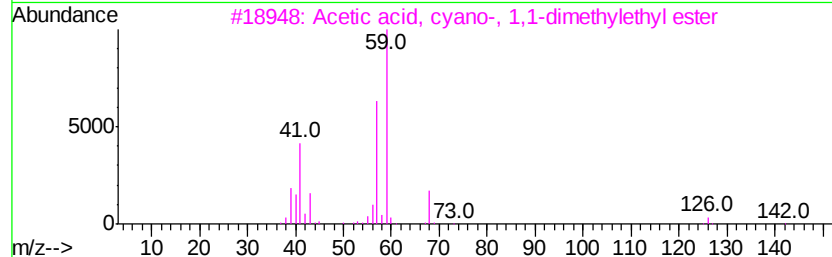
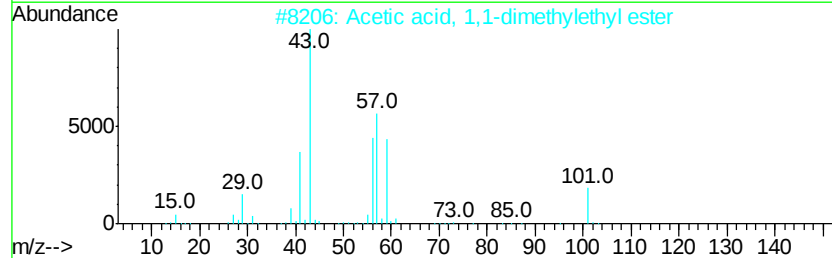
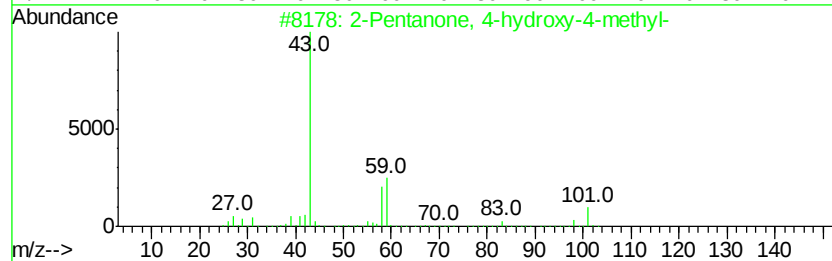
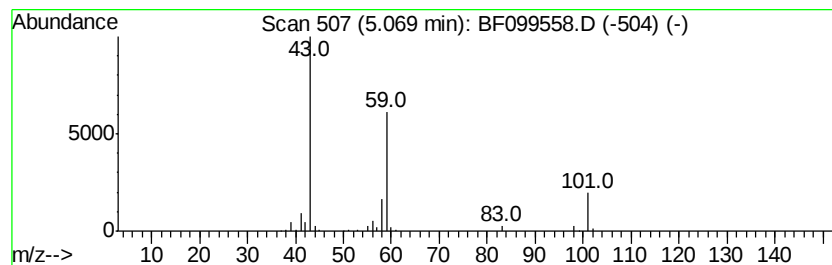
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.07	15.93 ng	469443	1,4-Dichlorobenzene-d4	6.85

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3			Acetic acid, cyano-, 1,1-dimethy...	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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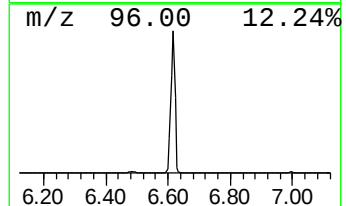
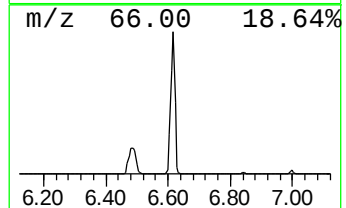
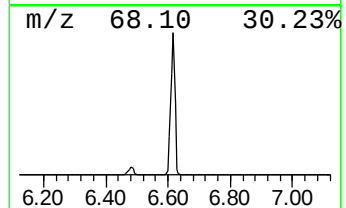
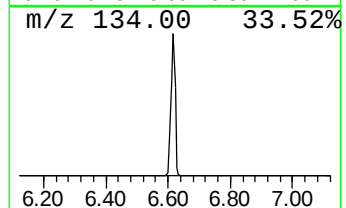
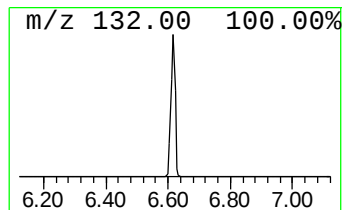
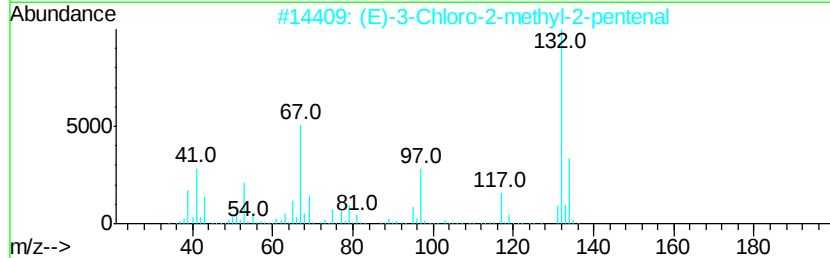
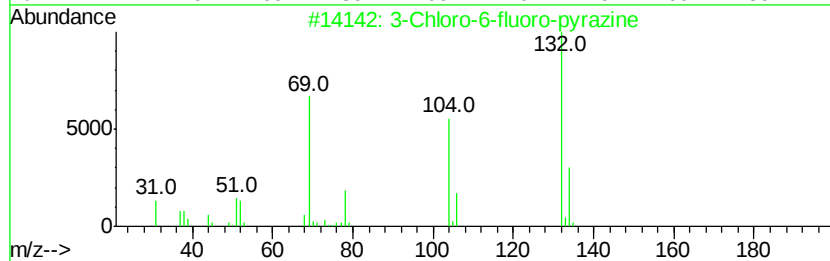
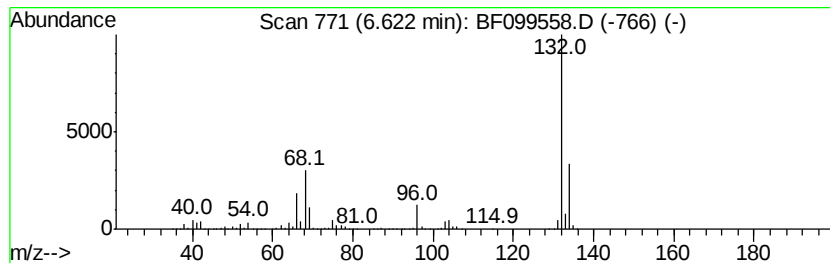
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Peak Number 2 unknown6.62 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.62	80.41 ng	2369000	1,4-Dichlorobenzene-d4	6.85

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	12
4		5-Aminoindole	132	C8H8N2	005192-03-0	12
5		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9



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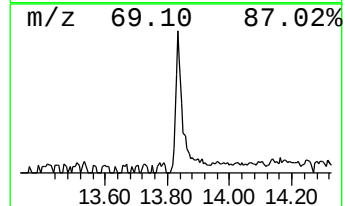
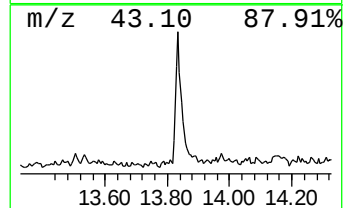
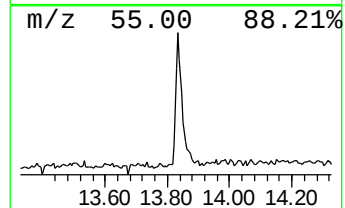
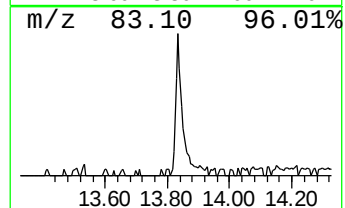
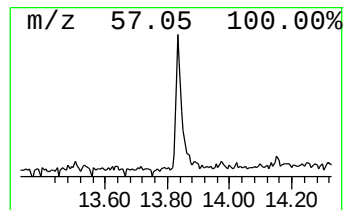
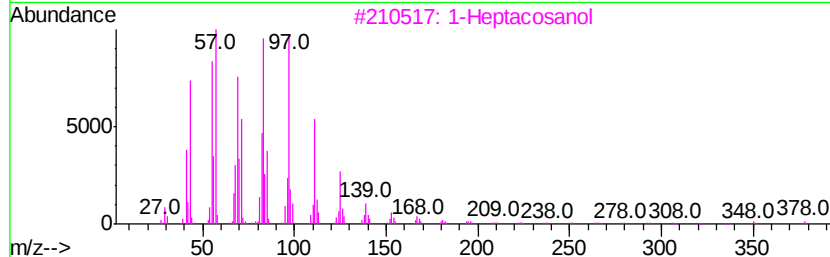
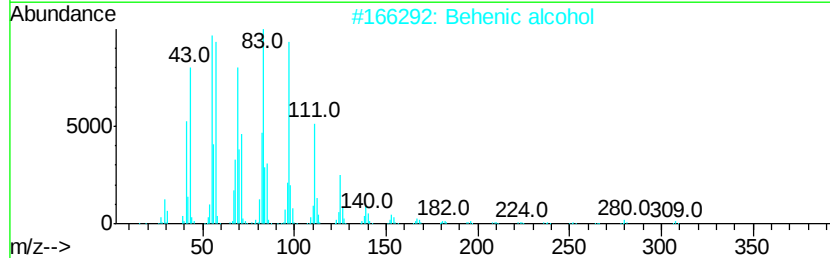
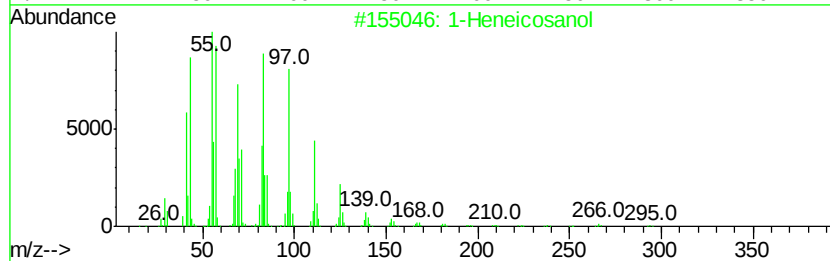
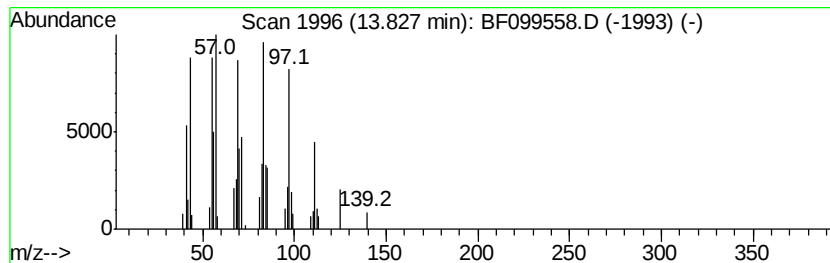
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Peak Number 4 1-Heneicosanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.		
13.83	4.65 ng	124390	Chrysene-d12	14.02		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Heneicosanol	312	C21H44O	015594-90-8	95
2		Behenic alcohol	326	C22H46O	000661-19-8	94
3		1-Heptacosanol	396	C27H56O	002004-39-9	94
4		Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	93
5		Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	93



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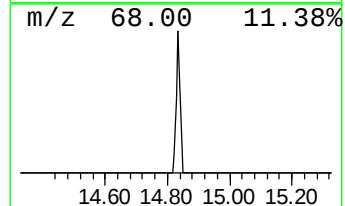
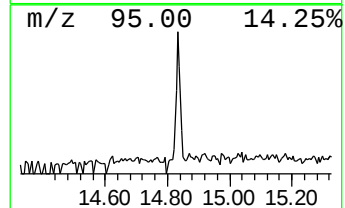
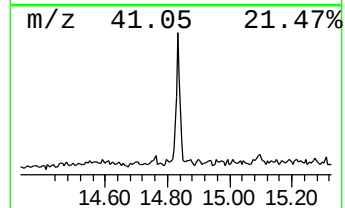
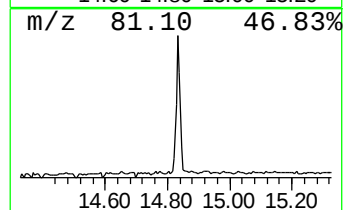
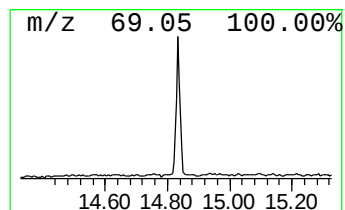
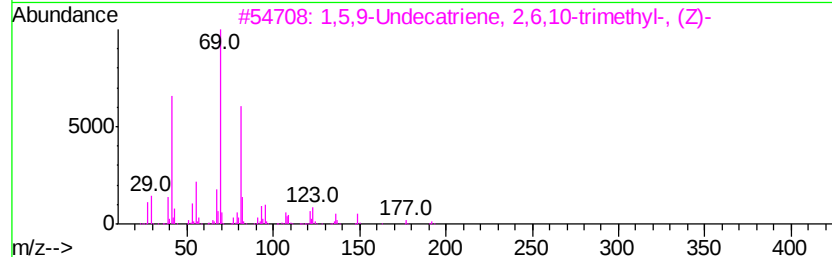
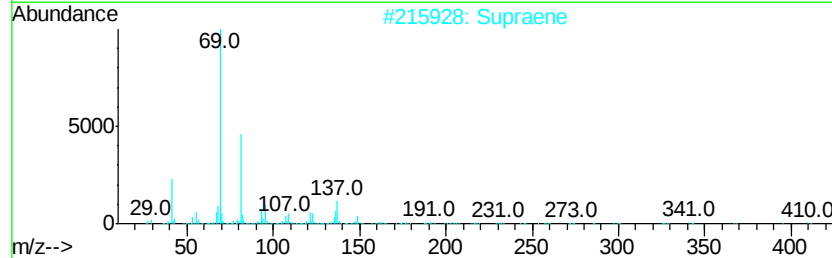
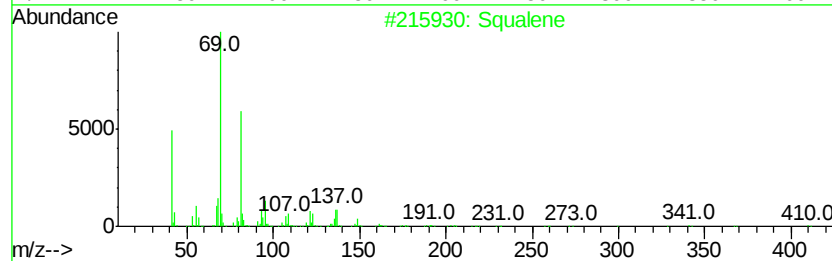
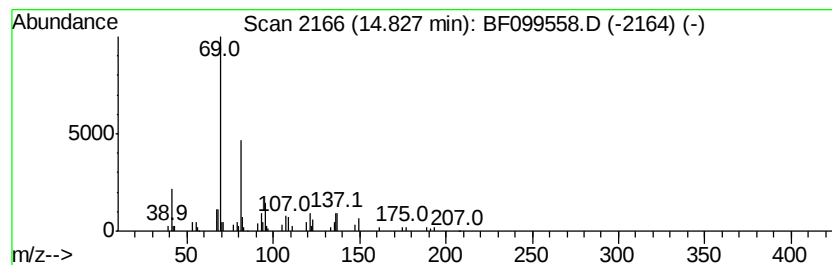
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Peak Number 5 Squalene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.83	3.77 ng	103660	Perylene-d12	15.49	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	91
2	Supraene	410	C30H50	007683-64-9	91
3	1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	87
4	Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	83
5	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	72



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.07	15.9	ng	469443	1	6.85	589204	20.0
unknown6.62	6.62	80.4	ng	2369000	1	6.85	589204	20.0
1-Heneicosanol	13.83	4.7	ng	124390	5	14.02	535512	20.0
Squalene	14.83	3.8	ng	103660	6	15.49	549233	20.0