

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF070618\
 Data File : BF107183.D
 Acq On : 6 Jul 2018 19:53
 Operator : JU/SJ
 Sample : J3854-03
 Misc :
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 S5

Integration Parameters: rteint.p
 Integrator: RTE
 Smoothing : ON
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0

Filtering: 5
 Min Area: 3 % of largest Peak
 Max Peaks: 100
 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-BF061918.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	5.184	480	484	503	rBB	139675	178975	14.02%	1.238%
2	5.589	548	553	584	rVB	1224359	1156516	90.61%	7.999%
3	6.595	718	724	741	rBV	1049486	1191294	93.33%	8.240%
4	6.725	741	746	751	rBV	1300207	1163380	91.14%	8.047%
5	6.942	779	783	790	rBB	397213	349388	27.37%	2.417%
6	7.101	805	810	823	rBB	1090713	941859	73.79%	6.515%
7	7.513	874	880	897	rBV	783455	747186	58.54%	5.168%
8	8.230	997	1002	1025	rVB	428161	445949	34.94%	3.084%
9	9.301	1178	1184	1192	rBV	1437482	1276428	100.00%	8.829%
10	9.695	1245	1251	1260	rBB	189817	174589	13.68%	1.208%
11	9.989	1294	1301	1311	rVB	463287	441135	34.56%	3.051%
12	10.783	1430	1436	1448	rBV	712997	671454	52.60%	4.644%
13	11.483	1550	1555	1565	rBV2	434781	462194	36.21%	3.197%
14	12.701	1757	1762	1770	rBV	198347	172820	13.54%	1.195%
15	12.930	1795	1801	1807	rBV	192339	203136	15.91%	1.405%
16	13.065	1815	1824	1834	rBV	1273773	1175888	92.12%	8.133%
17	13.260	1850	1857	1865	rBV2	37231	65848	5.16%	0.455%
18	13.607	1914	1916	1936	rBV8	13664	67154	5.26%	0.464%
19	13.942	1969	1973	1999	rBV5	74006	137495	10.77%	0.951%
20	14.136	1999	2006	2022	rBV2	530978	776360	60.82%	5.370%
21	14.959	2076	2146	2185	rBV2	35421	473089	37.06%	3.272%
22	15.212	2185	2189	2205	rVB2	101342	252621	19.79%	1.747%
23	15.324	2206	2208	2231	rVB4	26270	59152	4.63%	0.409%
24	15.536	2240	2244	2251	rBV	51075	67554	5.29%	0.467%
25	15.601	2251	2255	2262	rVV	77557	133931	10.49%	0.926%
26	15.671	2262	2267	2382	rVB	269378	804358	63.02%	5.563%
27	16.377	2383	2387	2459	rVB9	42158	222384	17.42%	1.538%
28	16.830	2459	2464	2529	rVB4	44444	165470	12.96%	1.145%
29	17.248	2529	2535	2613	rVB3	33308	65521	5.13%	0.453%
30	17.730	2613	2617	2827	rVB	29325	414684	32.49%	2.868%

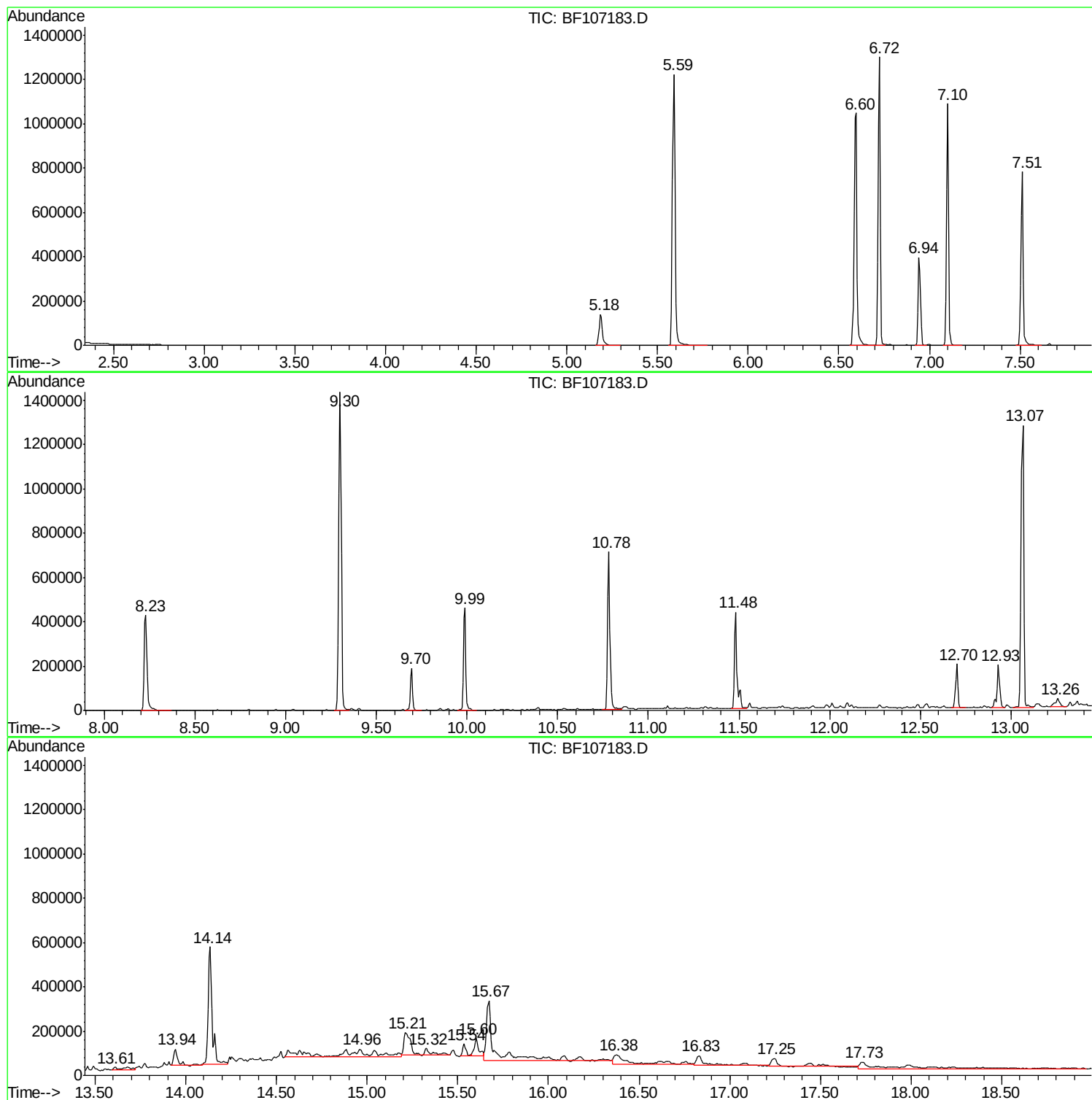
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ClientSampled :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF061918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: RTEINT.P



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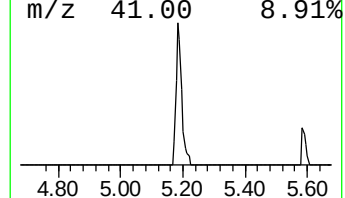
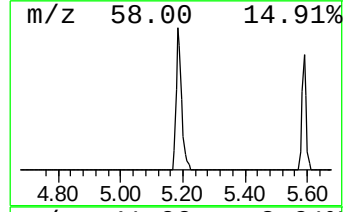
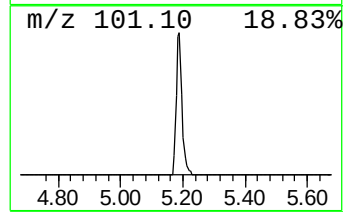
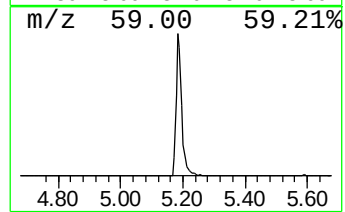
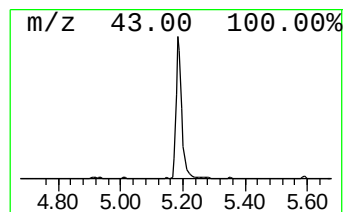
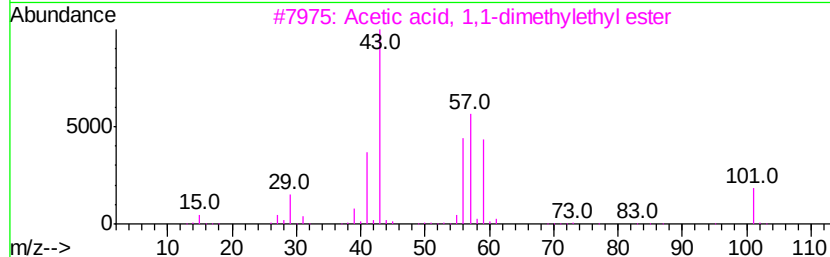
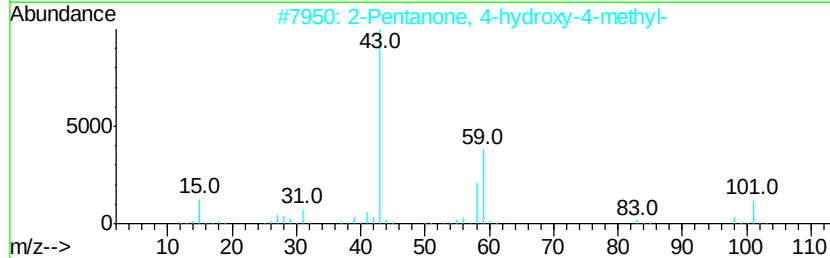
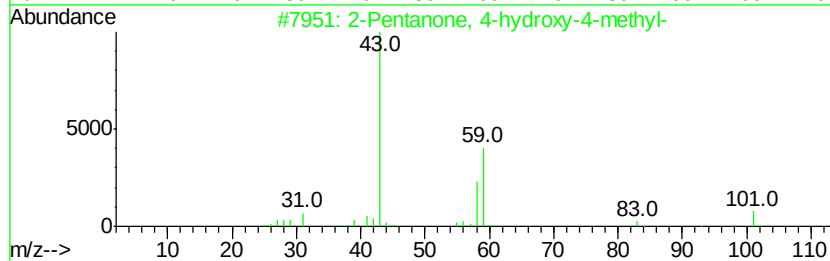
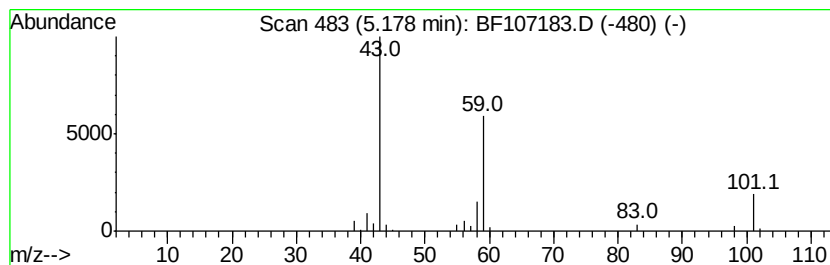
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: RTEINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.18	10.25 ng	178975	1,4-Dichlorobenzene-d4	6.94

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
3			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
4			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
5			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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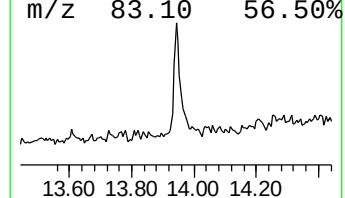
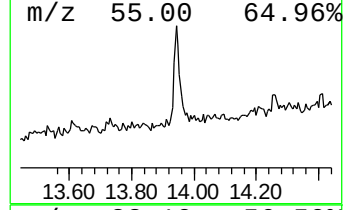
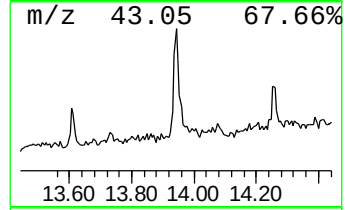
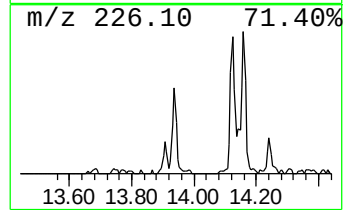
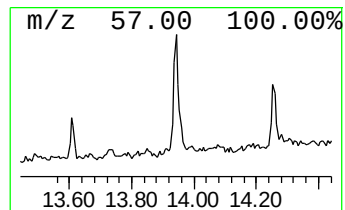
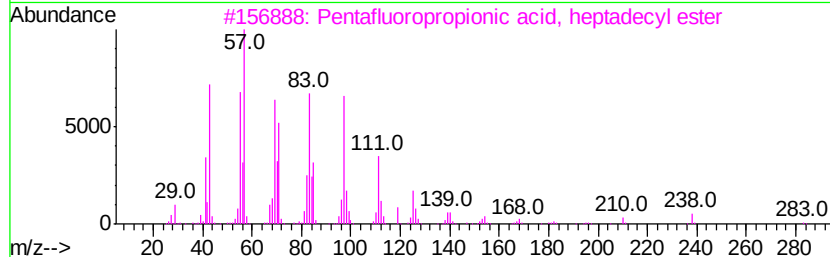
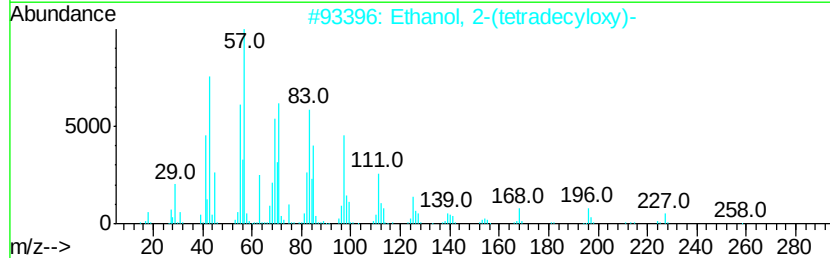
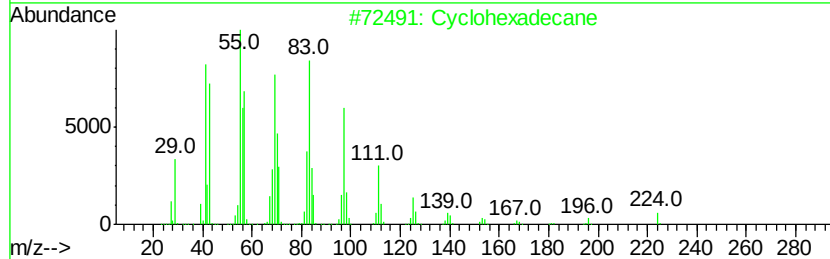
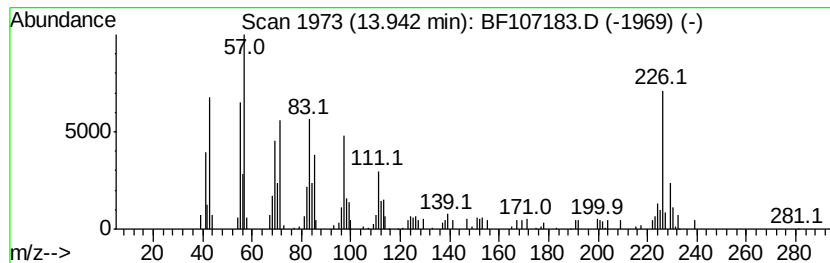
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Peak Number 2 Cyclohexadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.94	3.54 ng	137495	Chrysene-d12	14.14	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexadecane	224	C16H32	000295-65-8	87
2	Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	70
3	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	1000283-04-2	70
4	Heptafluorobutanoic acid, heptad...	452	C21H35F7O2	1000282-97-3	62
5	Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	62



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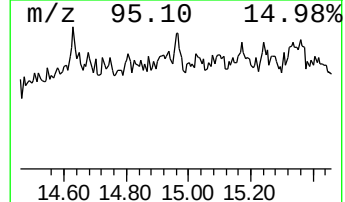
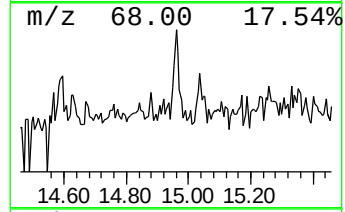
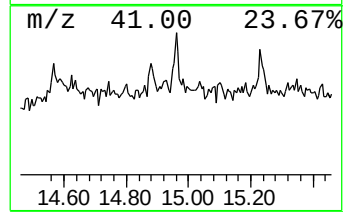
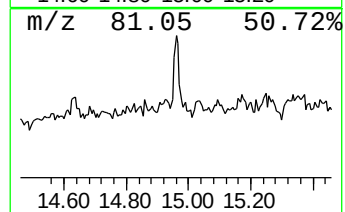
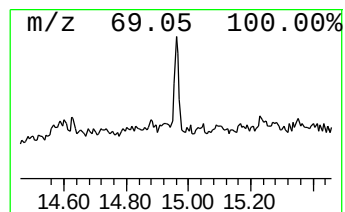
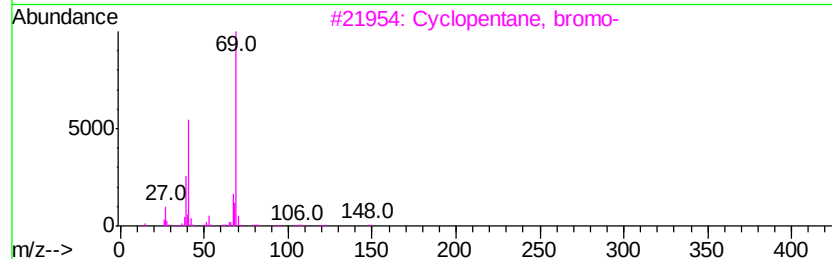
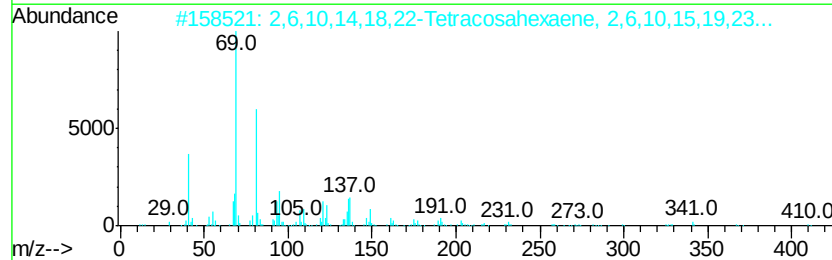
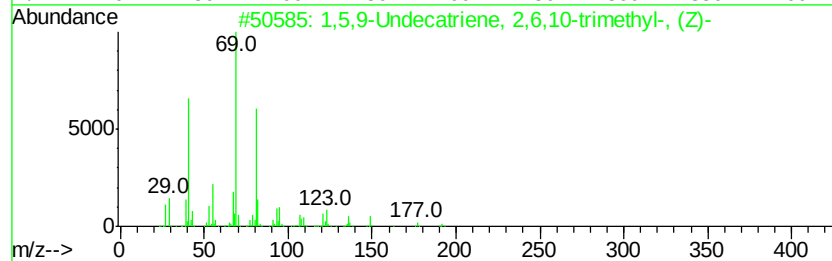
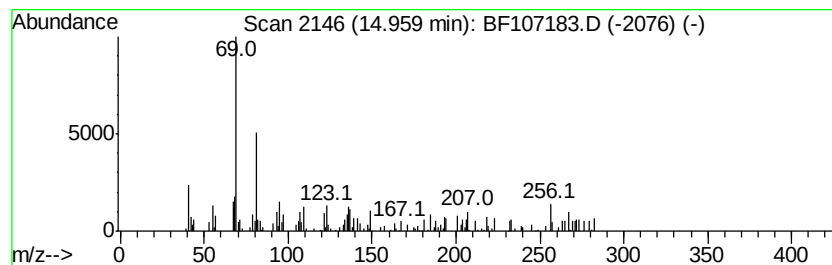
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Peak Number 3 1,5,9-Undecatriene, 2,6,10-... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.96	11.76 ng	473089	Perylene-d12	15.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	60
2		2,6,10,14,18,22-Tetracosahexaene...	410	C30H50	000111-02-4	49
3		Cyclopentane, bromo-	148	C5H9Br	000137-43-9	49
4		1,4-Hexadiene, 3,3,5-trimethyl-	124	C9H16	074753-00-7	49
5		2,6,10,14,18,22-Tetracosahexaene...	410	C30H50	000111-02-4	49



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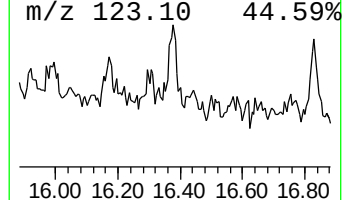
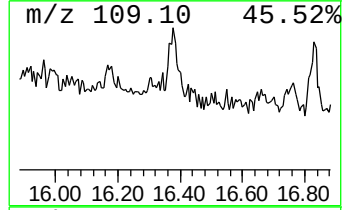
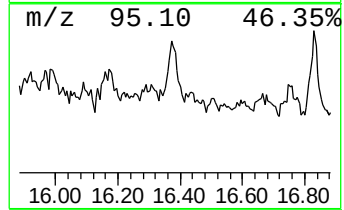
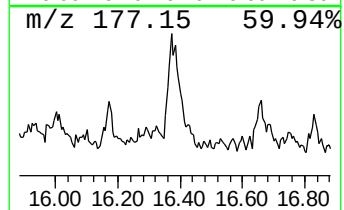
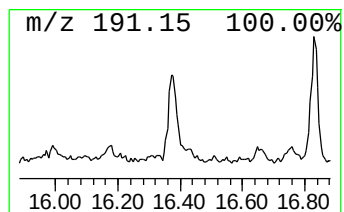
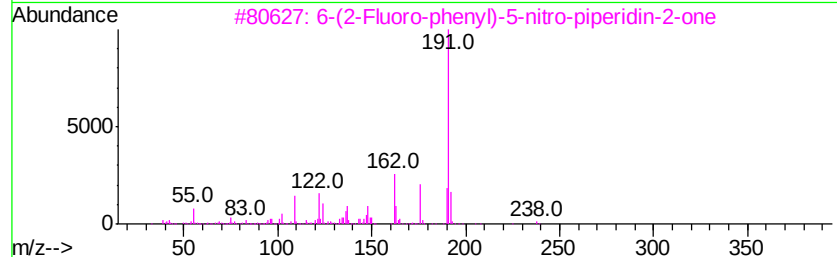
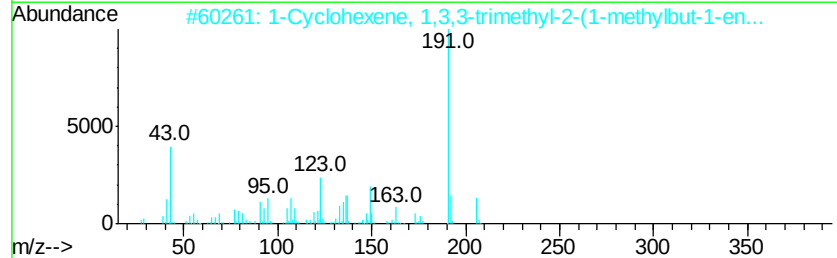
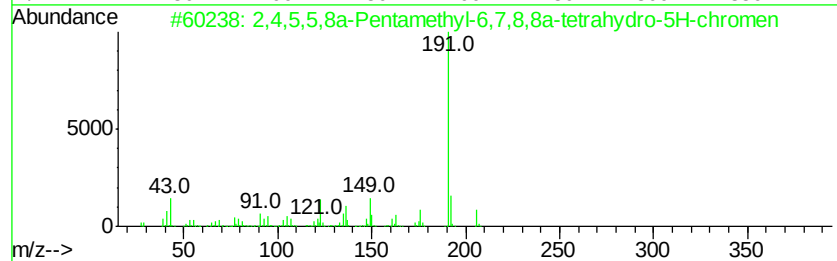
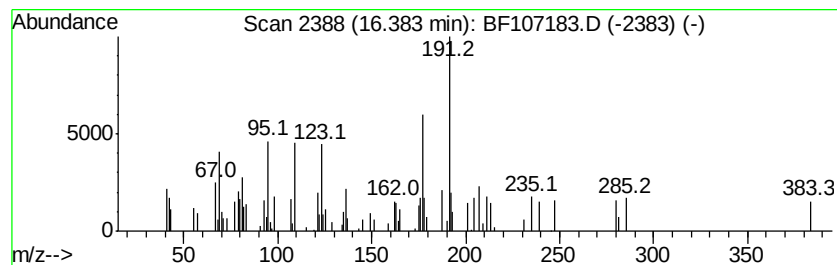
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Peak Number 4 2,4,5,5,8a-Pentamethyl-6,7,... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
16.38	5.53 ng	222384	Perylene-d12	15.67	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,5,5,8a-Pentamethyl-6,7,8,8a-...	206	C14H22O	1000195-40-9	60
2	1-Cyclohexene, 1,3,3-trimethyl-2...	206	C14H22O	1000197-08-4	43
3	6-(2-Fluoro-phenyl)-5-nitro-pipe...	238	C11H11FN2O3	1000275-16-4	43
4	1-Penten-3-one, 1-(2,6,6-trimeth...	206	C14H22O	000127-43-5	38
5	Propenamide, 3-(3,4-dimethoxyphe...	313	C18H19NO4	339165-72-9	32



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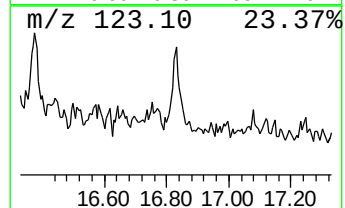
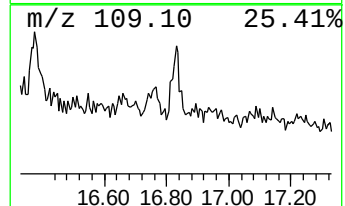
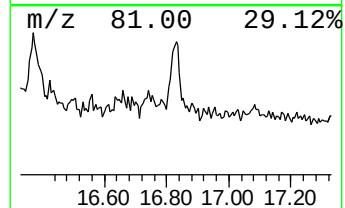
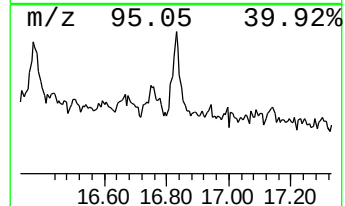
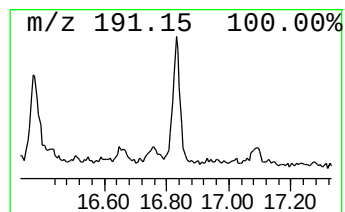
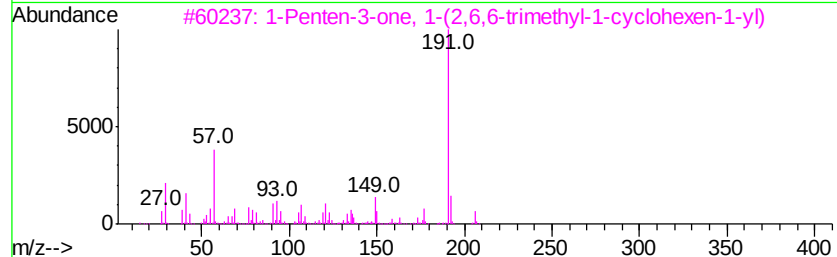
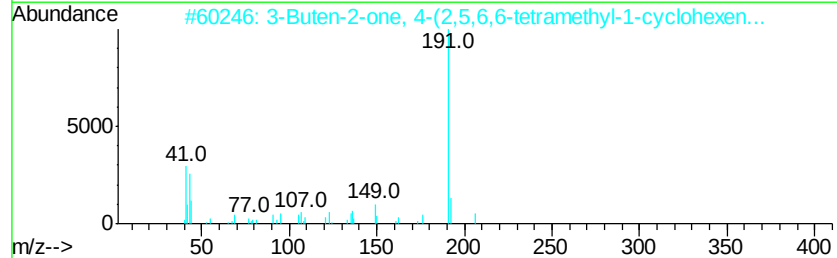
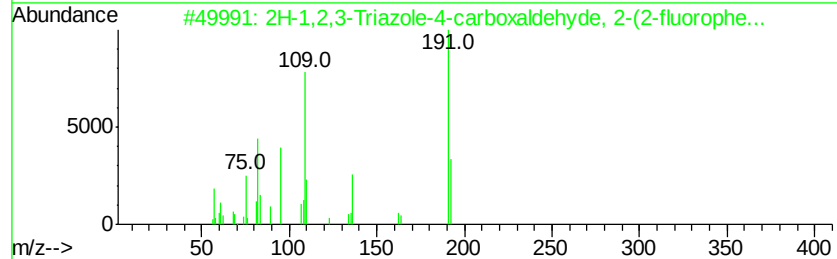
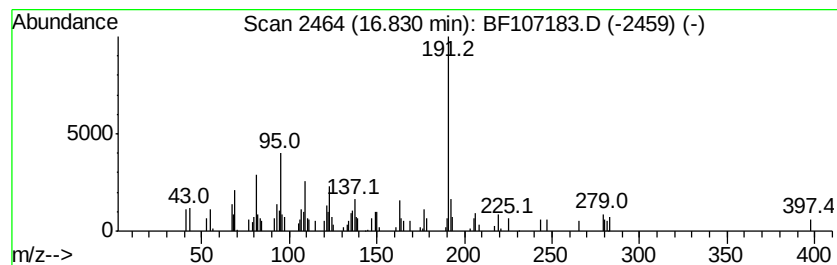
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Peak Number 5 unknown16.83 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.83	4.11 ng	165470	Perylene-d12	15.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2H-1,2,3-Triazole-4-carboxaldehy...	191	C9H6FN3O	051306-43-5	49
2		3-Buten-2-one, 4-(2,5,6,6-tetram...	206	C14H22O	000079-70-9	45
3		1-Penten-3-one, 1-(2,6,6-trimeth...	206	C14H22O	000127-43-5	45
4		4(1H)-Pteridinone, 2-amino-6,7-d...	191	C8H9N5O	000611-55-2	43
5		2,4,5,5,8a-Pentamethyl-6,7,8,8a-...	206	C14H22O	1000195-40-9	43



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.18	10.3	ng	178975	1	6.94	349388	20.0
Cyclohexadecane	13.94	3.5	ng	137495	5	14.14	776360	20.0
1,5,9-Undecatrien...	14.96	11.8	ng	473089	6	15.67	804358	20.0
2,4,5,5,8a-Pentam...	16.38	5.5	ng	222384	6	15.67	804358	20.0
unknown16.83	16.83	4.1	ng	165470	6	15.67	804358	20.0