

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051823\
 Data File : BF133444.D
 Acq On : 18 May 2023 18:11
 Operator : CG\JU
 Sample : 02828-02
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-2

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-BF042123.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF133444.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.899	473	478	488	rVB	935811	1196091	22.37%	3.242%
2	5.328	547	551	562	rBV	4538742	4238518	79.29%	11.490%
3	5.716	614	617	623	rVB	76058	73425	1.37%	0.199%
4	6.357	722	726	729	rBV	4086351	4163195	77.88%	11.286%
5	6.710	783	786	797	rBV	1430806	1127906	21.10%	3.058%
6	7.281	878	883	886	rBV	2864856	2734998	51.16%	7.414%
7	7.998	1001	1005	1010	rBV	1698901	1543636	28.88%	4.184%
8	9.075	1184	1188	1191	rBV	5841663	4981487	93.19%	13.504%
9	9.745	1299	1302	1306	rBV	2024579	1758674	32.90%	4.767%
10	10.463	1420	1424	1427	rBV	313092	274199	5.13%	0.743%
11	10.539	1433	1437	1440	rBV	3229353	2929011	54.79%	7.940%
12	11.228	1551	1554	1560	rBV	1925098	1806789	33.80%	4.898%
13	11.769	1642	1646	1649	rBV	92760	109293	2.04%	0.296%
14	12.716	1802	1807	1814	rBV3	29608	61388	1.15%	0.166%
15	12.822	1820	1825	1827	rBV	5608534	5345665	100.00%	14.491%
16	12.845	1827	1829	1833	rVB	1064198	826903	15.47%	2.242%
17	13.363	1913	1917	1920	rBV	91277	77020	1.44%	0.209%
18	13.739	1974	1981	1987	rBV6	106596	340130	6.36%	0.922%
19	13.869	1999	2003	2010	rVB	1603254	1411650	26.41%	3.827%
20	14.045	2029	2033	2036	rBV	66314	62737	1.17%	0.170%
21	14.345	2078	2084	2089	rBV2	65048	91708	1.72%	0.249%
22	14.645	2131	2135	2142	rBV2	35899	65421	1.22%	0.177%
23	14.710	2143	2146	2155	rVB	188424	205170	3.84%	0.556%
24	15.286	2239	2244	2256	rBV	1063192	1350189	25.26%	3.660%
25	15.727	2315	2319	2324	rBV2	42358	58163	1.09%	0.158%
26	16.198	2395	2399	2403	rBV3	33293	56365	1.05%	0.153%

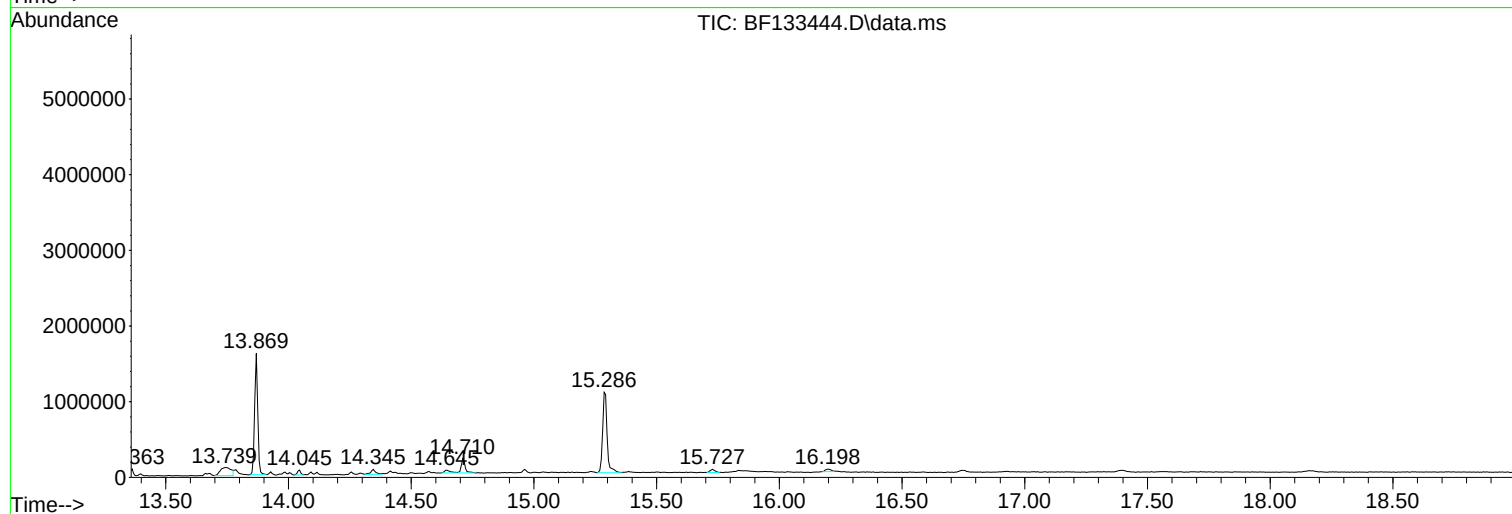
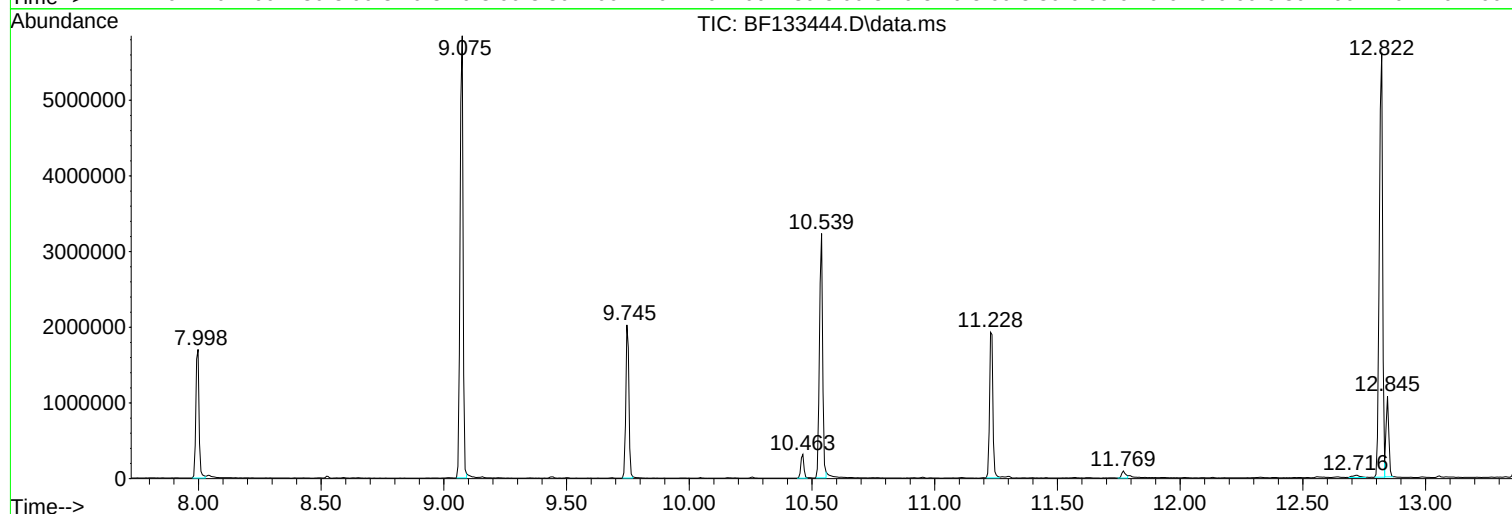
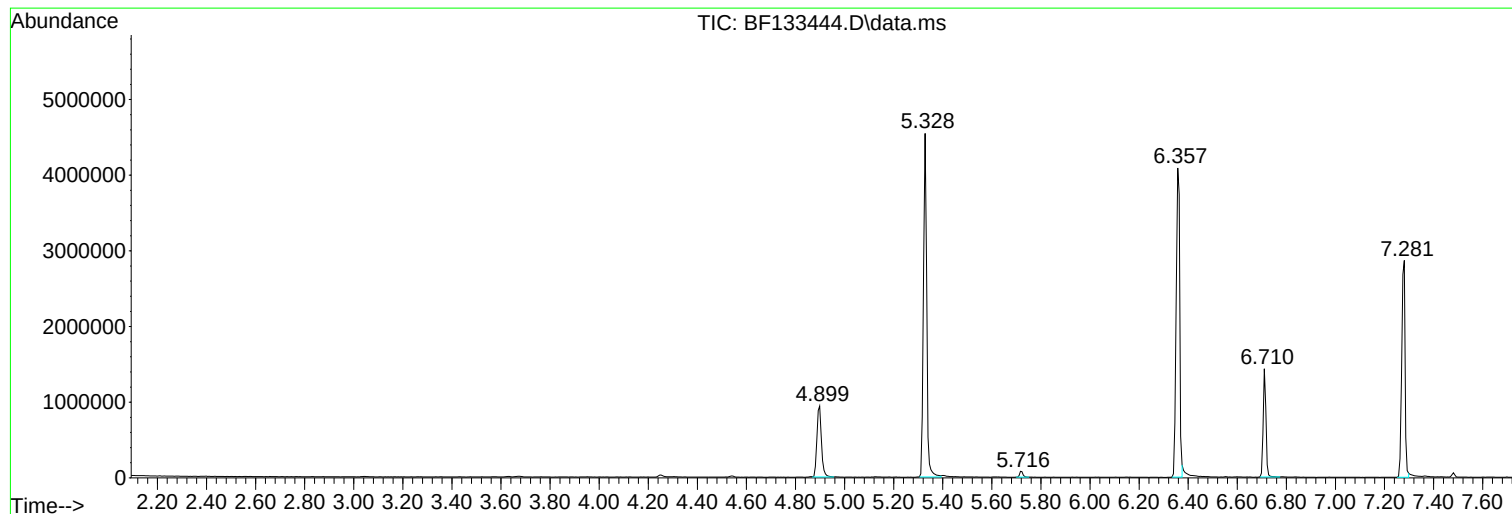
Sum of corrected areas: 36889731

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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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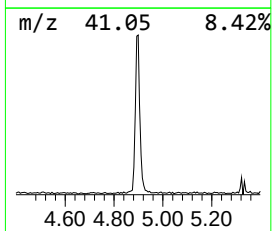
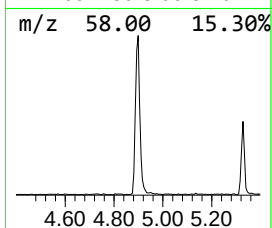
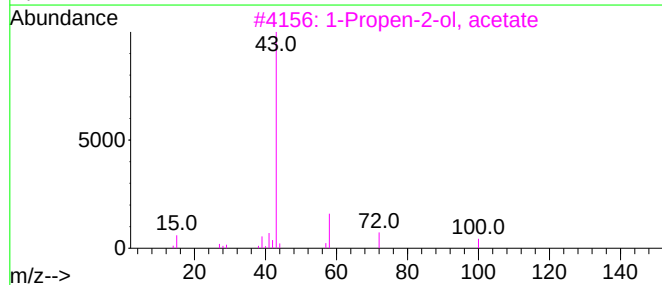
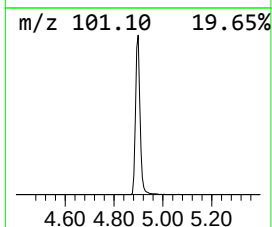
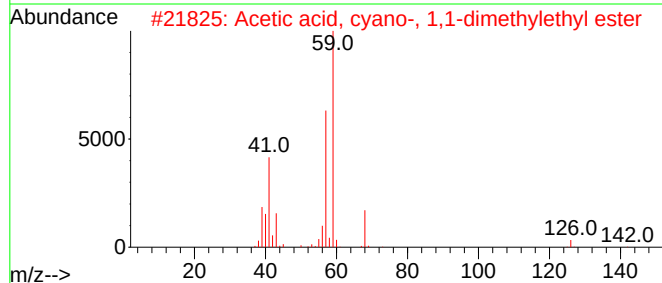
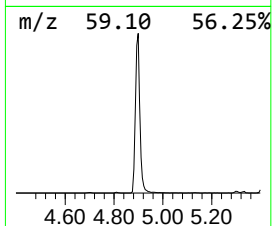
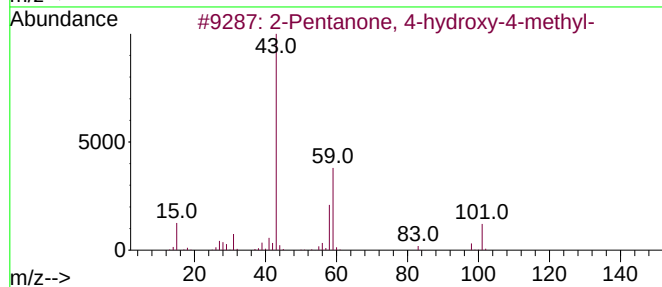
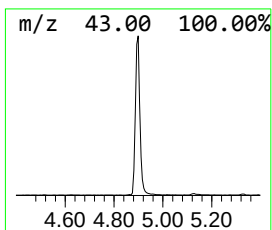
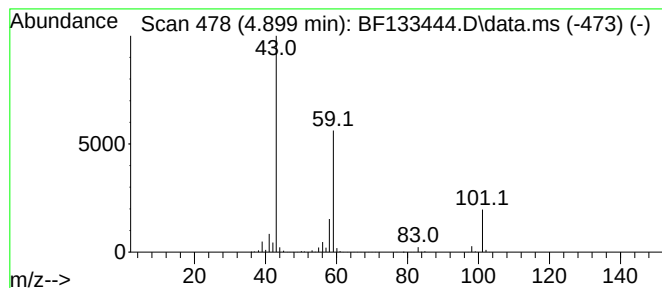
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.899	21.21 ng	1196090	1,4-Dichlorobenzene-d4	6.710

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	47		
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17		
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10		
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9		
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9		



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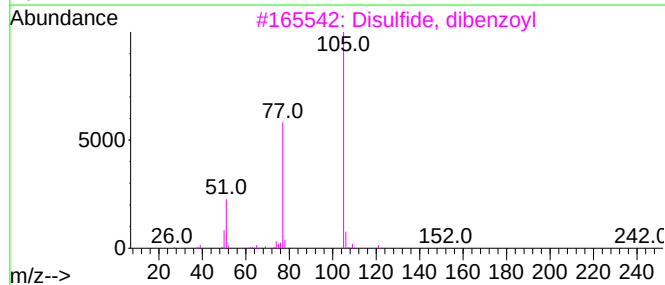
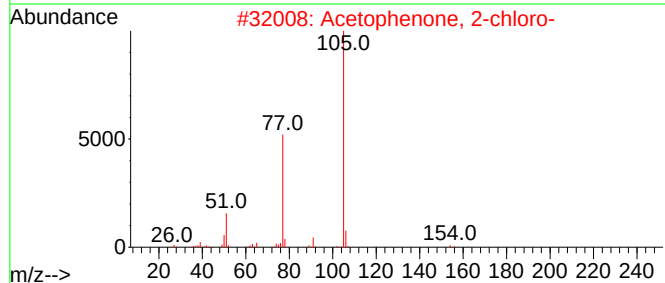
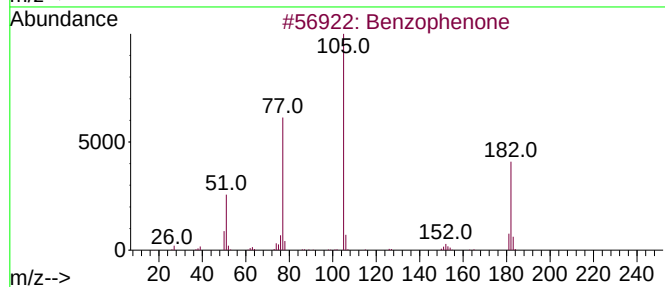
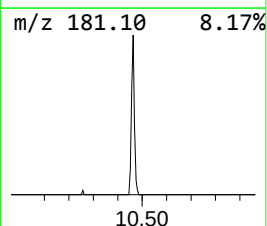
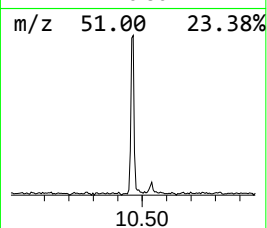
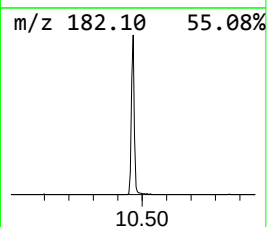
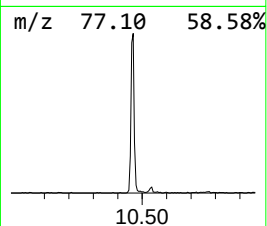
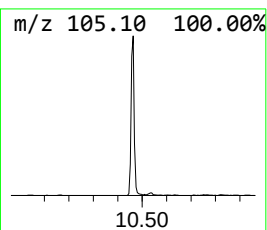
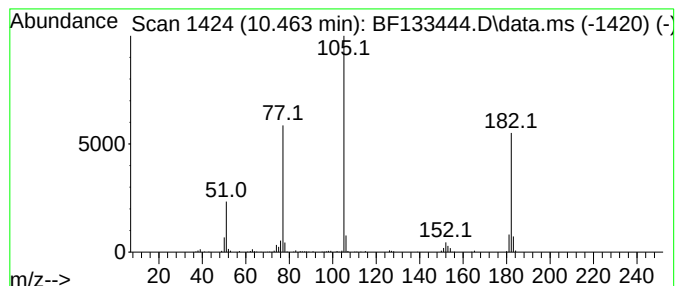
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Peak Number 2 Benzophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.463	3.12 ng	274199	Acenaphthene-d10	9.745

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	97
2			Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	49
3			Disulfide, dibenzoyl	274	C14H10O2S2	000644-32-6	49
4			1,2-Propanedione, 1-phenyl-	148	C9H8O2	000579-07-7	47
5			N-(1-Cyanovinyl)benzamide	172	C10H8N2O	1000186-19-1	47



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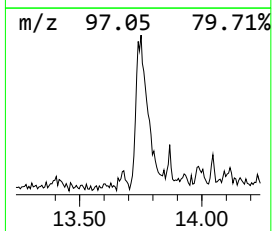
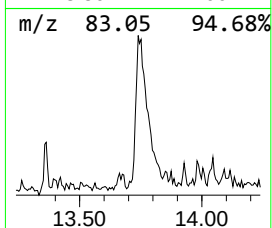
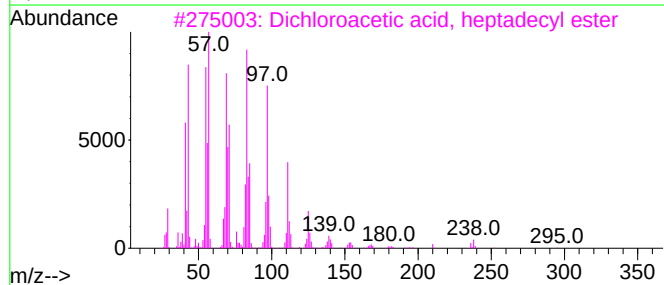
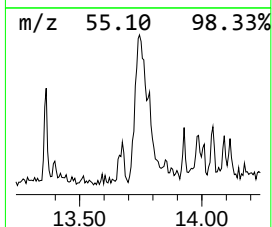
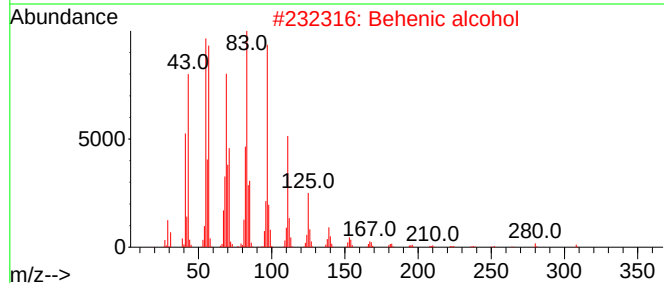
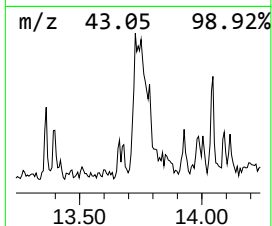
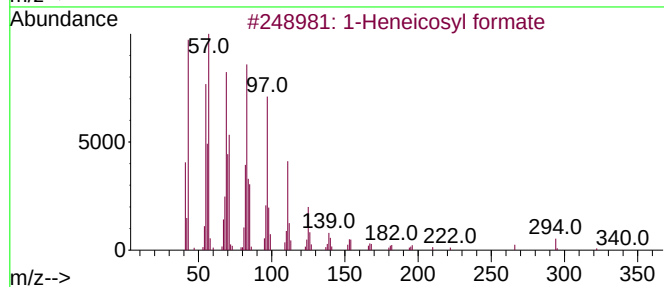
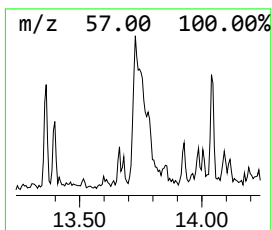
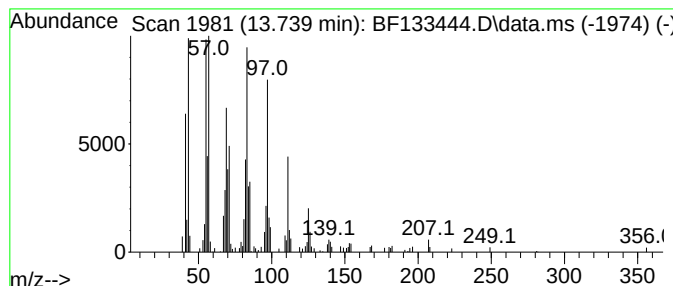
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Peak Number 3 1-Heneicosyl formate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.739	4.82 ng	340130	Chrysene-d12	13.868

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Heneicosyl formate	340	C22H44O2	077899-03-7	94
2			Behenic alcohol	326	C22H46O	000661-19-8	94
3			Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	94
4			1-Heneicosanol	312	C21H44O	015594-90-8	93
5			Octacosanol	410	C28H58O	000557-61-9	91



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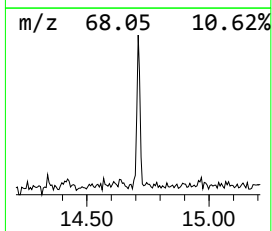
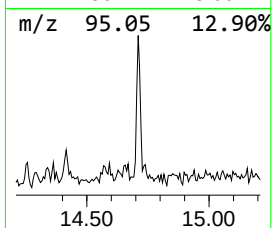
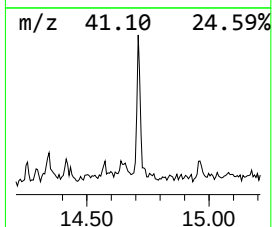
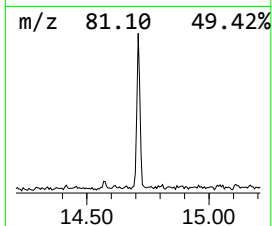
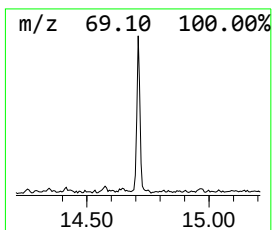
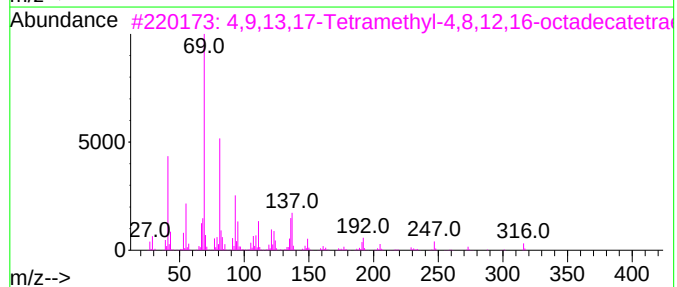
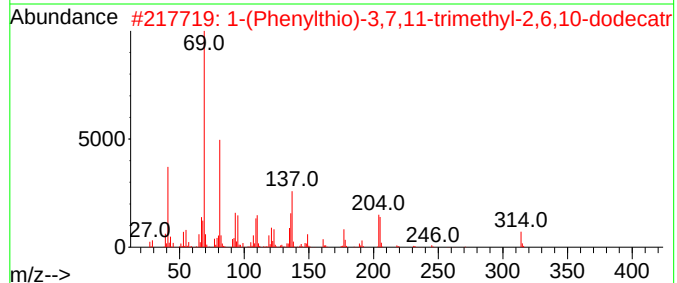
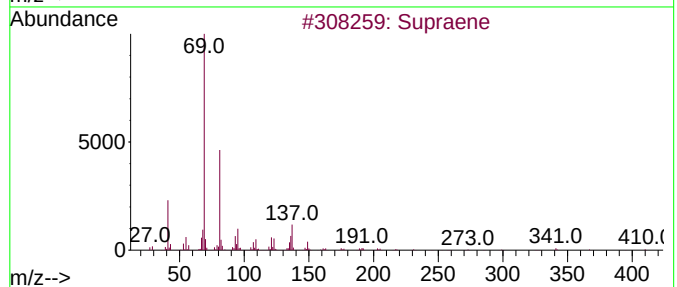
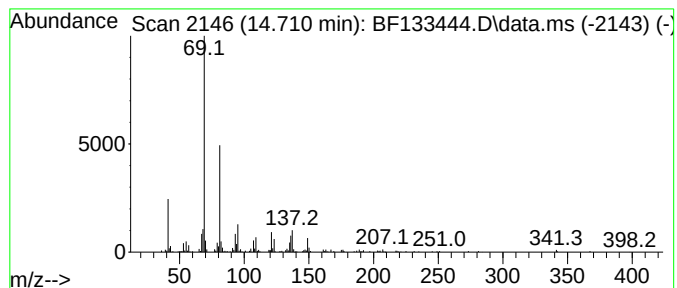
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Peak Number 4 Supraene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.710	3.04 ng	205170	Perylene-d12	15.286

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Supraene	410	C30H50	007683-64-9	91
2			1-(Phenylthio)-3,7,11-trimethyl-...	314	C21H30S	028413-57-2	78
3			4,9,13,17-Tetramethyl-4,8,12,16-...	316	C22H36O	056882-09-8	74
4			(.+/-)-Lavandulol, pentafluorop...	300	C13H17F5O2	1000352-63-1	64
5			3,7-Dimethyl-1-phenylsulfonyl-2,...	278	C16H22O2S	1000432-27-5	59



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	4.899	21.2	ng	1196090	1	6.710	1127910	20.0
Benzophenone	10.463	3.1	ng	274199	3	9.745	1758670	20.0
1-Heneicosyl fo...	13.739	4.8	ng	340130	5	13.868	1411650	20.0
Supraene	14.710	3.0	ng	205170	6	15.286	1350190	20.0