

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111121\
 Data File : BF126139.D
 Acq On : 11 Nov 2021 22:31
 Operator : JU/CG
 Sample : M4628-01
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 LAMINGTON-COMP

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-BF110321.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF126139.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.451	568	572	576	rBV	3089914	3046450	78.71%	11.878%
2	6.469	740	745	748	rBV	3538388	3182225	82.21%	12.407%
3	6.840	804	808	811	rBV	1141777	849063	21.94%	3.310%
4	7.398	899	903	906	rBV	2157051	2050135	52.97%	7.993%
5	8.028	1006	1010	1022	rBV	375038	416644	10.76%	1.624%
6	8.122	1022	1026	1030	rVB	1325873	1076626	27.81%	4.198%
7	9.198	1205	1209	1212	rBV	4722661	3870684	100.00%	15.091%
8	9.875	1321	1324	1328	rBV	1432432	1243330	32.12%	4.848%
9	10.663	1454	1458	1462	rBV	2867923	2335116	60.33%	9.104%
10	11.363	1573	1577	1580	rBV	1463783	1160773	29.99%	4.526%
11	12.951	1842	1847	1850	rBV	3585720	3239165	83.68%	12.629%
12	13.233	1891	1895	1902	rBV	43514	50254	1.30%	0.196%
13	13.880	1998	2005	2015	rBV7	59708	146126	3.78%	0.570%
14	13.998	2021	2025	2029	rBV	1081324	1041783	26.91%	4.062%
15	14.386	2087	2091	2094	rBV	38138	53464	1.38%	0.208%
16	14.763	2152	2155	2162	rBV	169200	192031	4.96%	0.749%
17	14.863	2168	2172	2175	rBV	128853	133062	3.44%	0.519%
18	15.339	2249	2253	2257	rBV	79577	93184	2.41%	0.363%
19	15.398	2260	2263	2269	rVV	47919	65798	1.70%	0.257%
20	15.462	2270	2274	2279	rVV	816862	1003194	25.92%	3.911%
21	15.504	2279	2281	2287	rVB6	36614	55526	1.43%	0.216%
22	15.815	2331	2334	2340	rVB	48159	70280	1.82%	0.274%
23	15.945	2352	2356	2361	rBV2	51534	75815	1.96%	0.296%
24	16.451	2438	2442	2449	rVB8	45415	83278	2.15%	0.325%
25	17.045	2538	2543	2546	rBV5	29750	44899	1.16%	0.175%
26	17.345	2591	2594	2600	rVB4	37437	69621	1.80%	0.271%

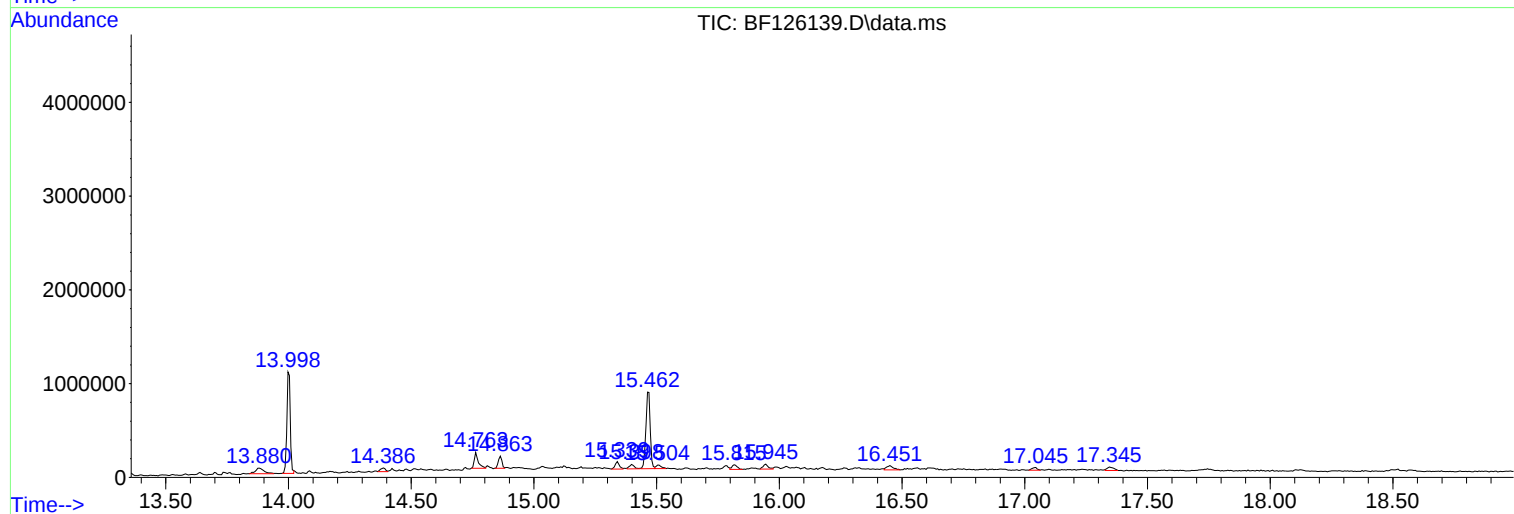
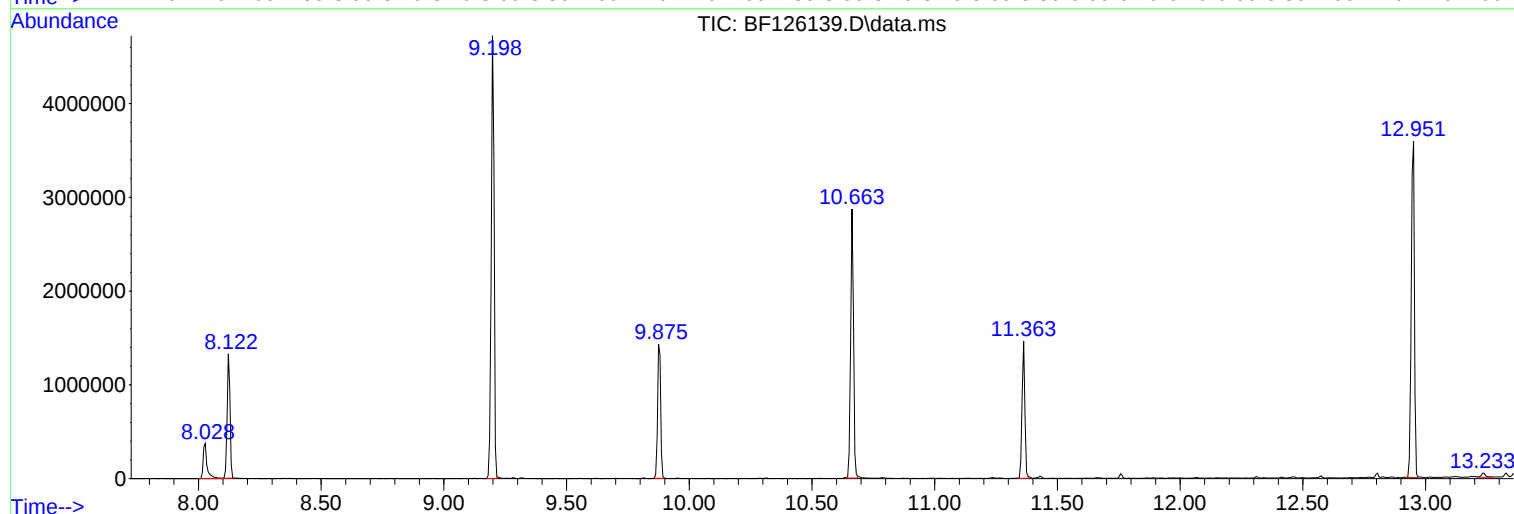
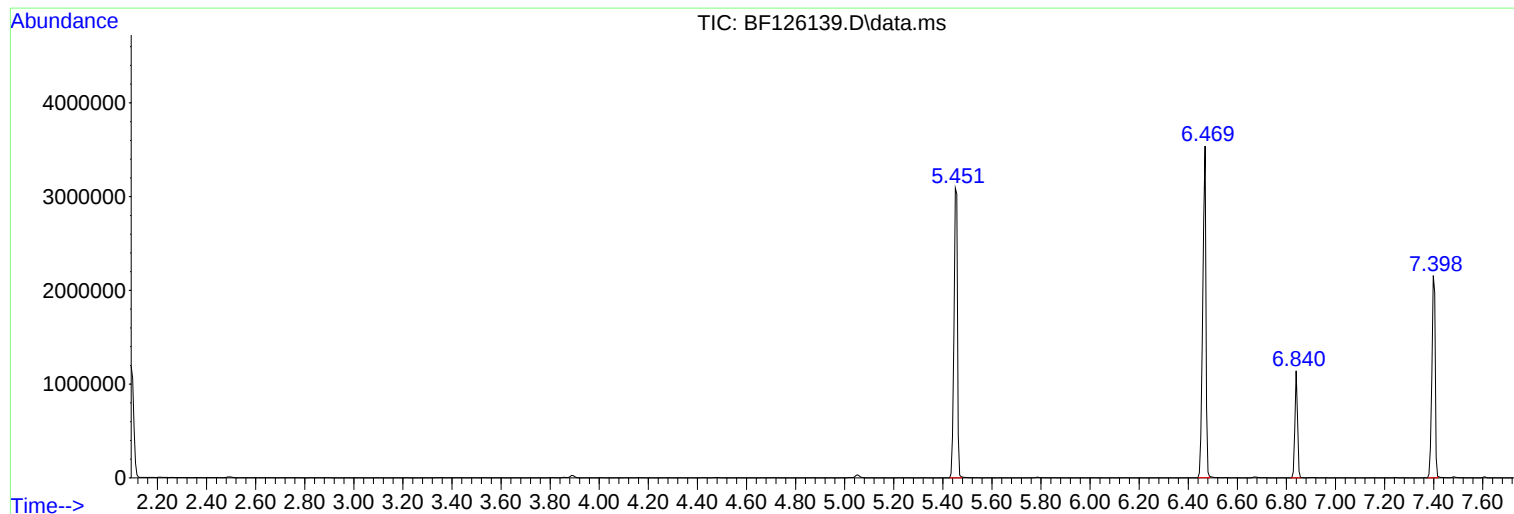
Sum of corrected areas: 25648526

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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110321.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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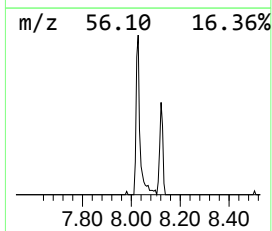
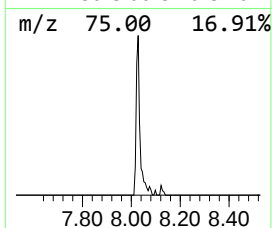
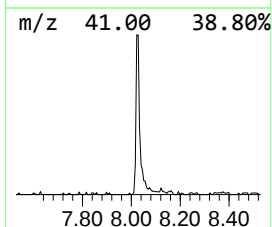
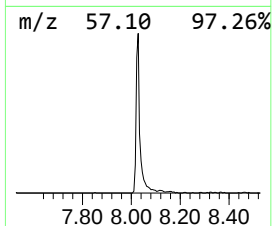
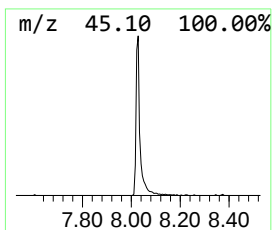
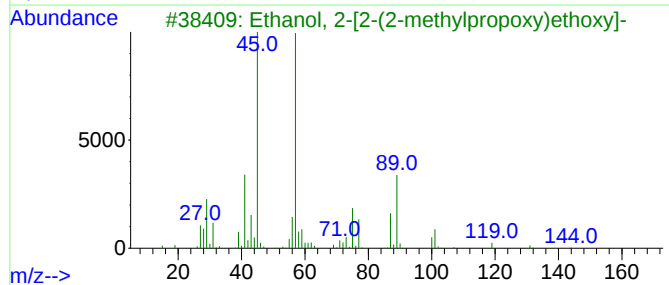
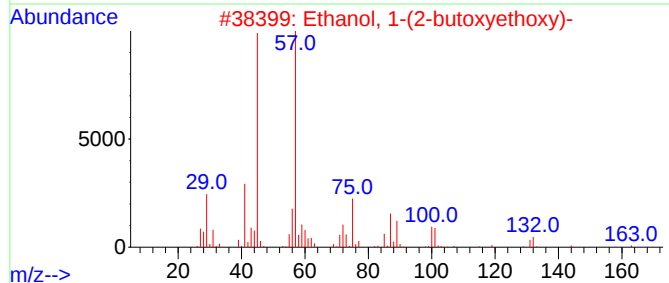
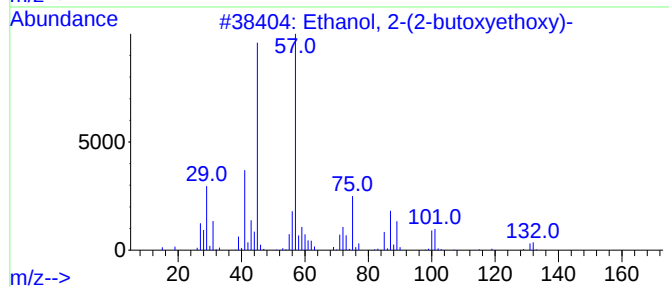
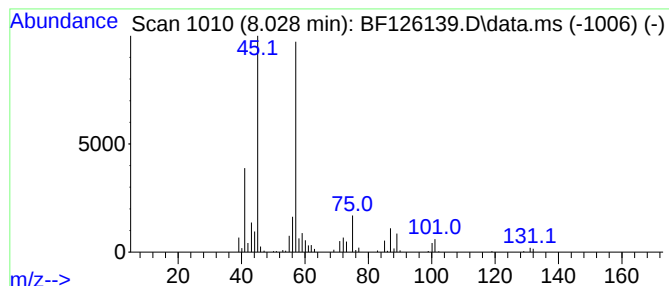
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.028	7.74 ng	416644	Naphthalene-d8	8.122

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2			Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	83
3			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	78
4			Di-sec-Butyl ether	130	C8H18O	006863-58-7	59
5			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	50



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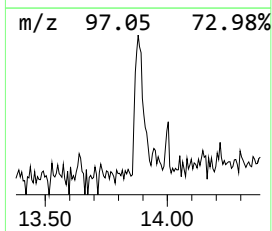
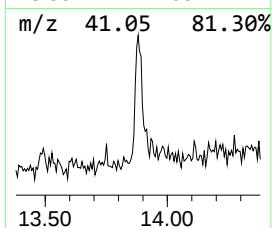
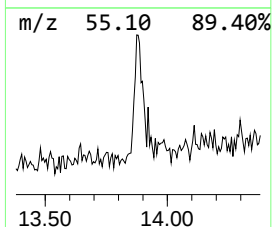
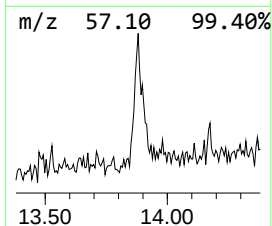
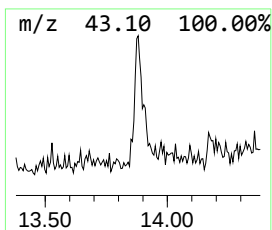
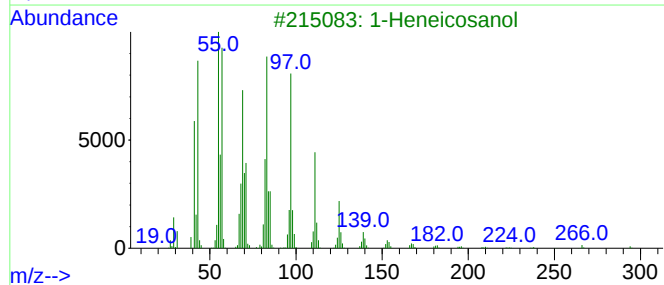
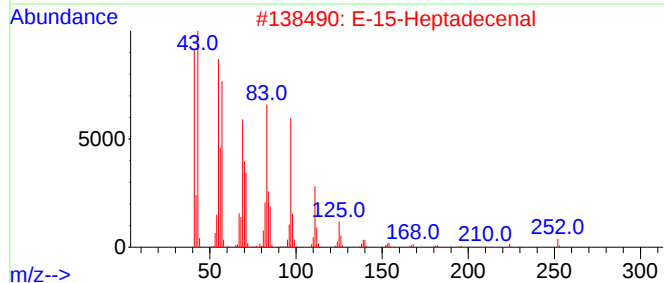
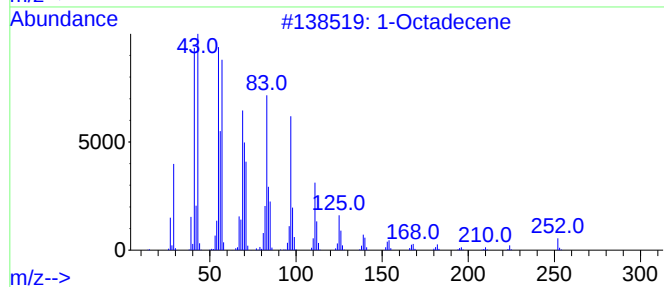
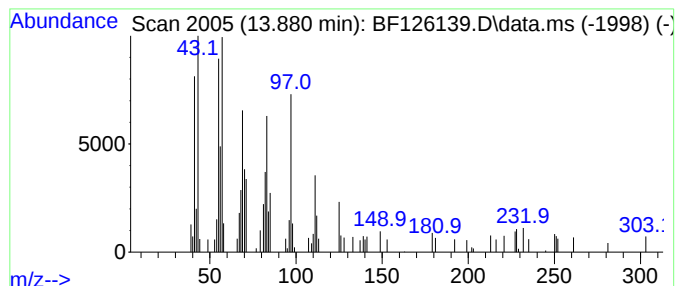
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Peak Number 2 1-Octadecene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.880	2.81 ng	146126	Chrysene-d12	13.998

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Octadecene			252	C18H36	000112-88-9	93
2	E-15-Heptadecenal			252	C17H32O	1000130-97-9	90
3	1-Heneicosanol			312	C21H44O	015594-90-8	90
4	1-Tricosene			322	C23H46	018835-32-0	87
5	1-Docosene			308	C22H44	001599-67-3	83



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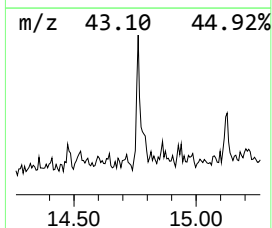
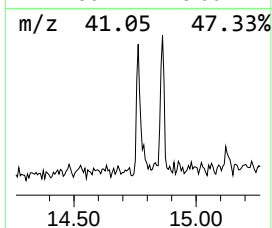
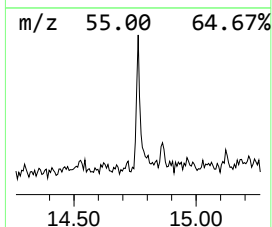
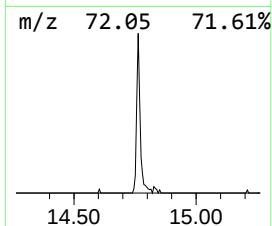
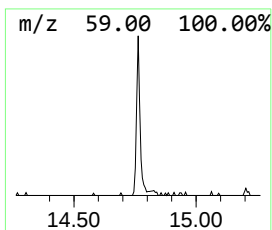
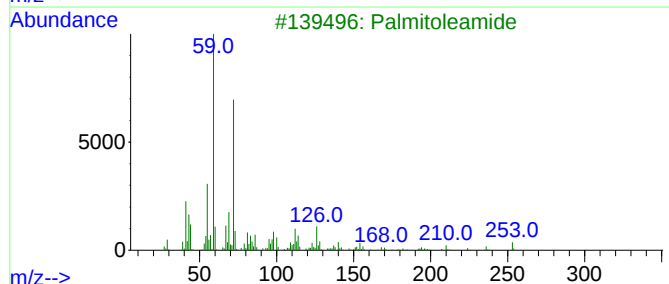
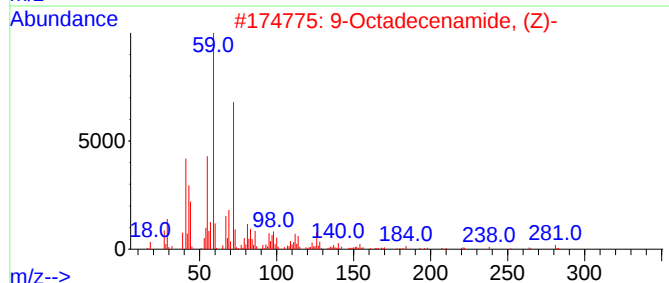
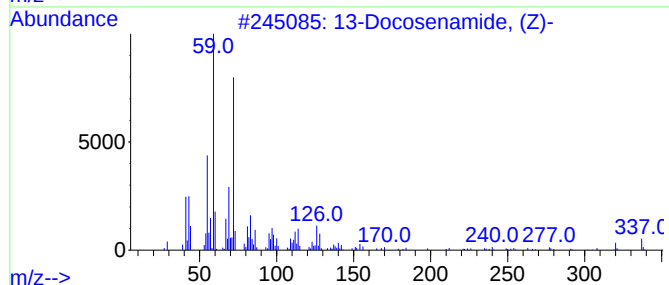
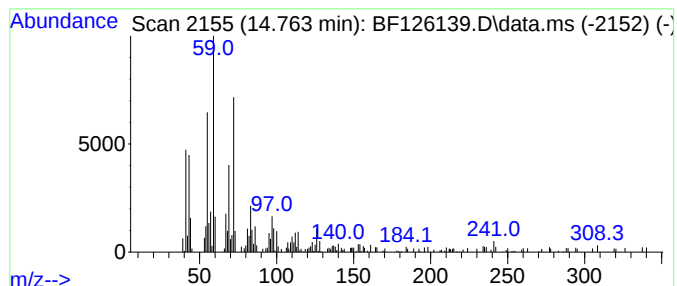
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Peak Number 3 13-Docosenamide, (Z)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.762	3.83 ng	192031	Perylene-d12	15.468

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	94
2			9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	91
3			Palmitoleamide	253	C16H31NO	106010-22-4	83
4			Dodecanamide	199	C12H25NO	001120-16-7	49
5			Benzeneethanamine, 2-fluoro-.bet...	229	C11H16FN03	061338-98-5	49



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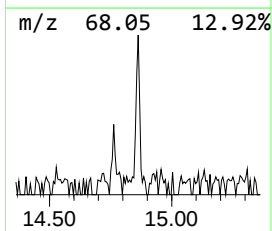
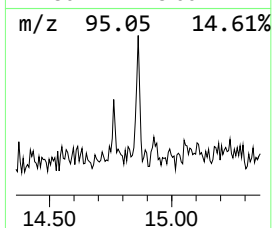
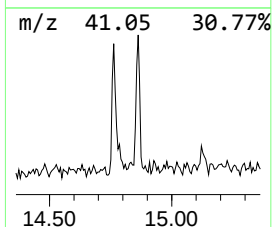
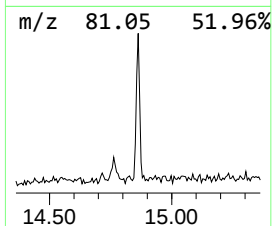
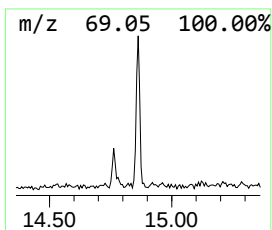
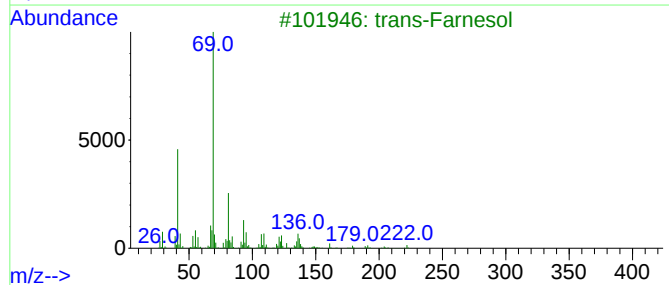
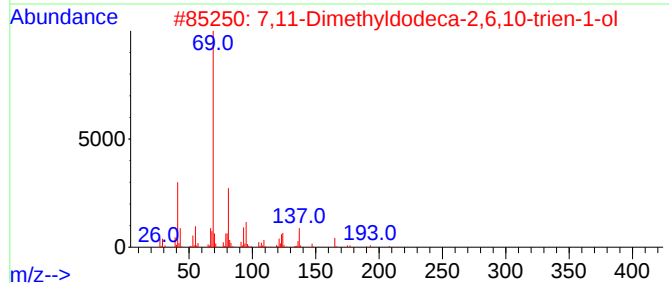
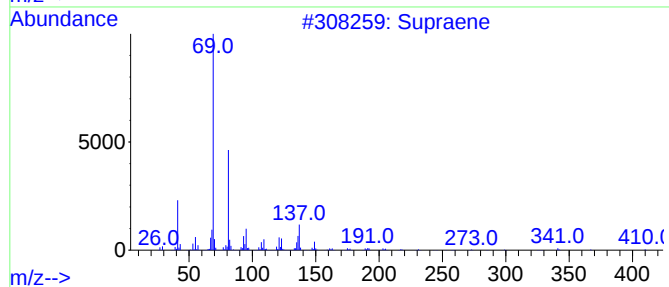
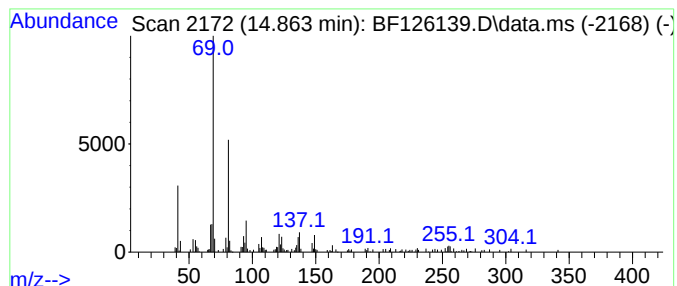
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Peak Number 4 Supraene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.863	2.65 ng	133062	Perylene-d12	15.468

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Supraene	410	C30H50	007683-64-9	80
2			7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	80
3			trans-Farnesol	222	C15H26O	000106-28-5	72
4			(3E,7E)-4,8,12-Trimethyltrideca...	218	C16H26	062235-06-7	72
5			5,9,13,17-Tetramethyl 4,8,12,16-...	332	C22H36O2	1000432-37-9	72



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Ethanol, 2-(2-b...	8.028	7.7	ng	416644	2	8.122	1076630	20.0
1-Octadecene	13.880	2.8	ng	146126	5	13.998	1041780	20.0
13-Docosenamide...	14.762	3.8	ng	192031	6	15.468	1003190	20.0
Supraene	14.863	2.6	ng	133062	6	15.468	1003190	20.0