

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111121\
 Data File : BF126128.D
 Acq On : 11 Nov 2021 16:34
 Operator : JU/CG
 Sample : M4635-01
 Misc :
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 VWE-B20-11921-0-10

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: BF126128.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.457	568	573	576	rBV	4332309	4185683	68.53%	11.878%
2	6.469	740	745	748	rBV	4085190	4346191	71.16%	12.333%
3	6.839	805	808	812	rBV	1143169	866717	14.19%	2.459%
4	7.404	898	904	907	rBV	3214903	2803634	45.90%	7.956%
5	8.028	1006	1010	1022	rBV	728688	702135	11.50%	1.992%
6	8.122	1022	1026	1030	rVV	1282524	1113085	18.22%	3.159%
7	9.204	1205	1210	1213	rBV	6208142	5432125	88.94%	15.415%
8	9.880	1321	1325	1328	rBV	1535955	1343820	22.00%	3.813%
9	10.669	1454	1459	1462	rBV	4197771	3737565	61.19%	10.606%
10	11.363	1573	1577	1581	rBV	1827774	1464103	23.97%	4.155%
11	11.433	1583	1589	1592	rVB5	69020	70804	1.16%	0.201%
12	12.951	1843	1847	1850	rBV	6223638	6107750	100.00%	17.332%
13	13.880	1999	2005	2015	rBV3	138608	309405	5.07%	0.878%
14	14.004	2019	2026	2029	rBV	1306067	1152697	18.87%	3.271%
15	14.639	2130	2134	2138	rBV	331744	297986	4.88%	0.846%
16	14.862	2168	2172	2175	rBV	136837	133570	2.19%	0.379%
17	15.468	2270	2275	2279	rBV	836342	994304	16.28%	2.822%
18	15.945	2351	2356	2361	rVB	67430	104363	1.71%	0.296%
19	18.168	2730	2734	2743	rVB	31769	74306	1.22%	0.211%

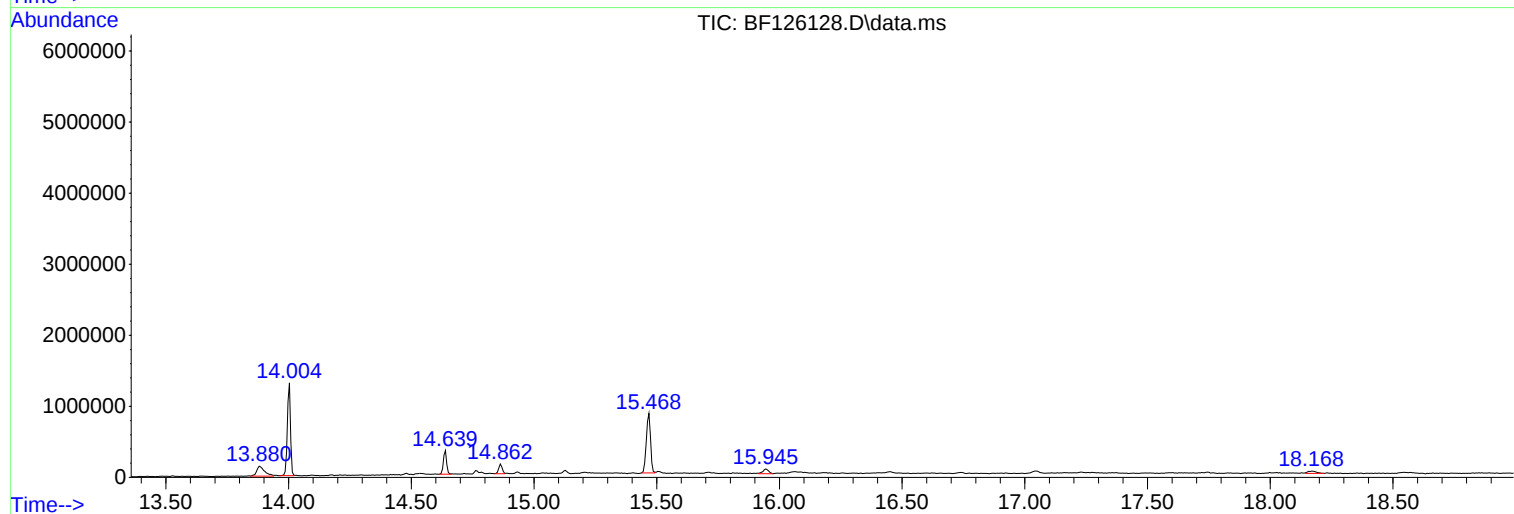
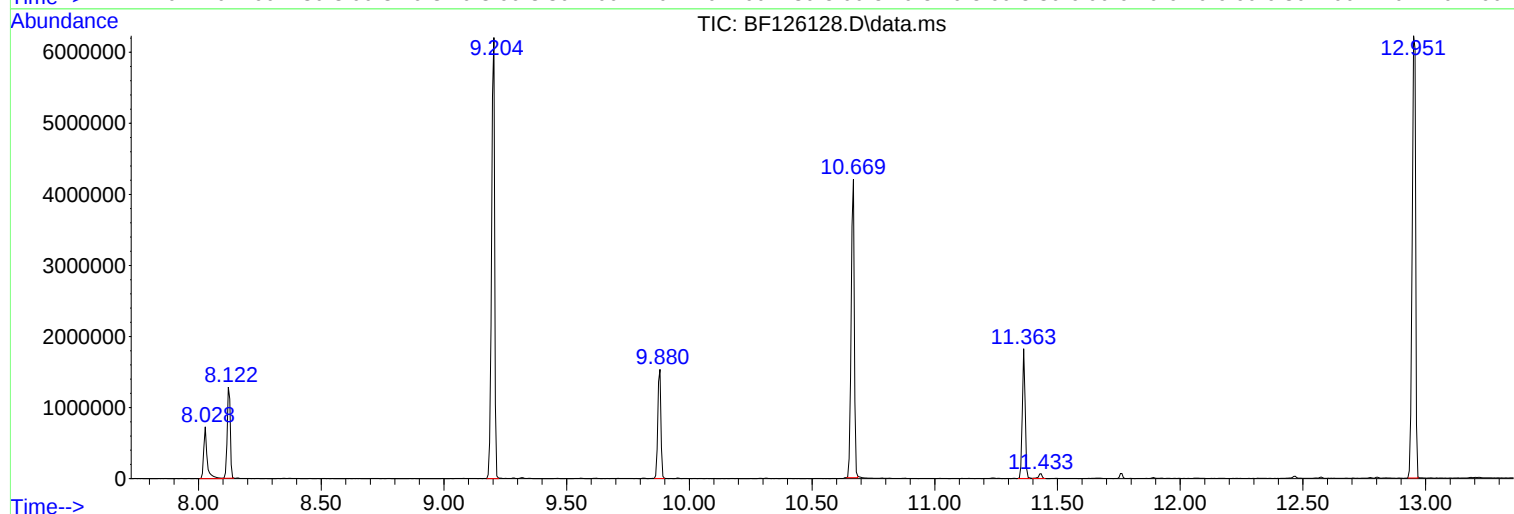
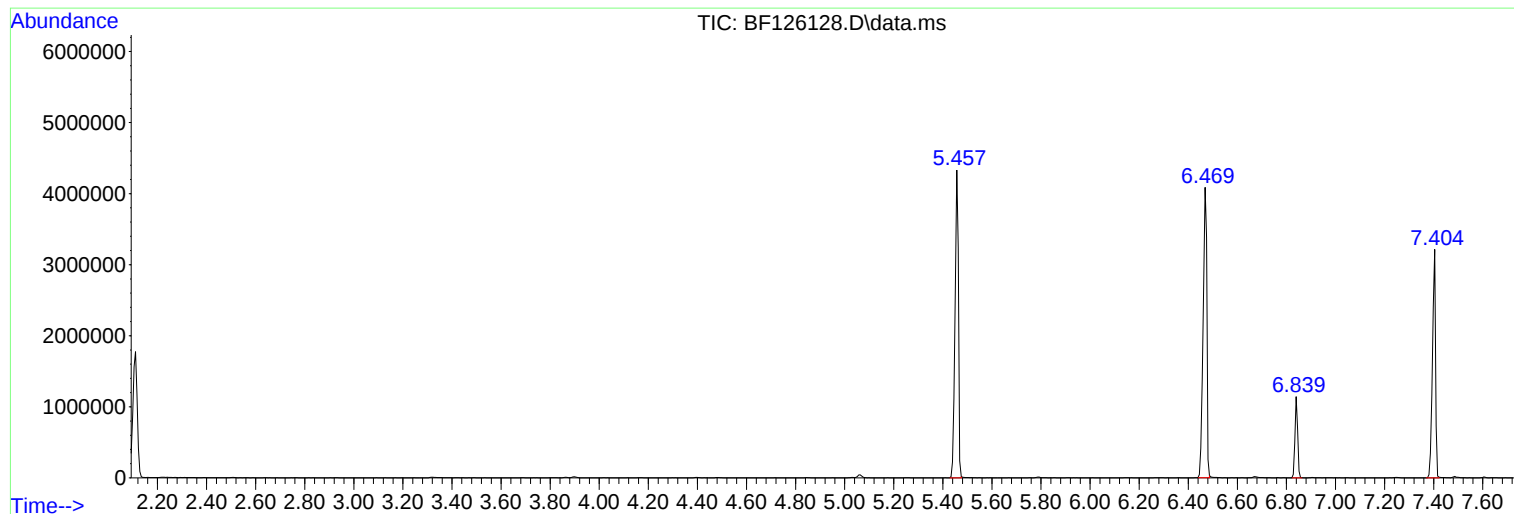
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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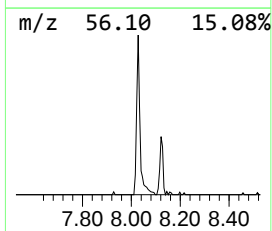
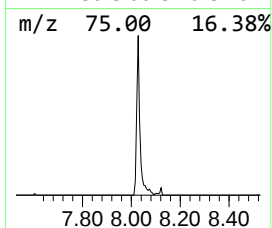
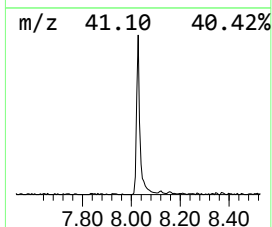
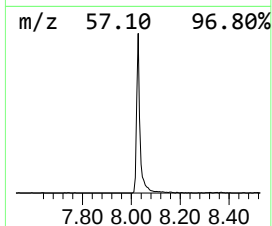
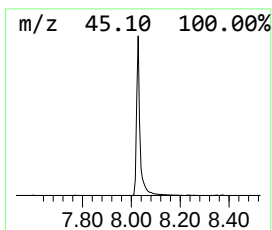
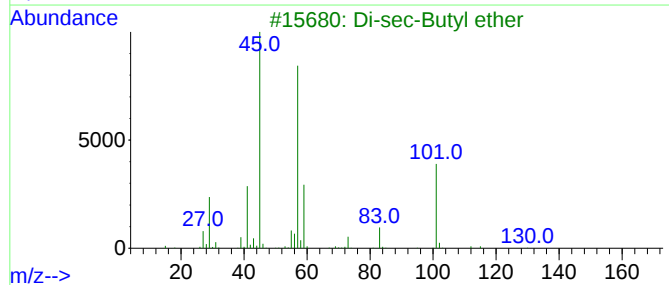
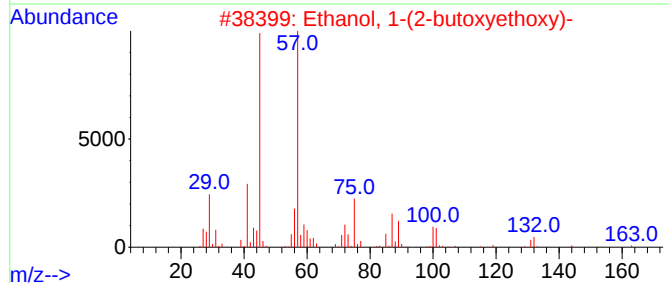
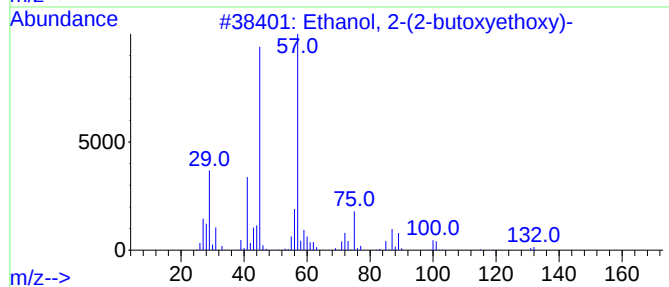
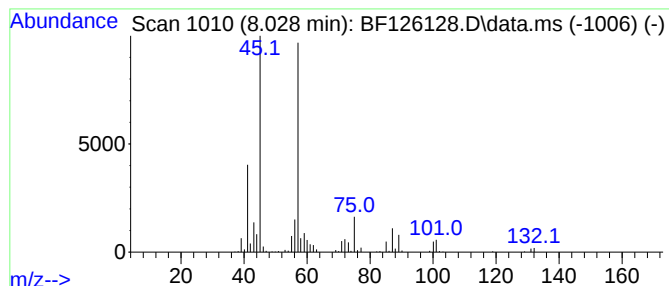
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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	12.62 ng	702135	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			Di-sec-Butyl ether	130	C8H18O	006863-58-7	53
4			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	50
5			3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	50



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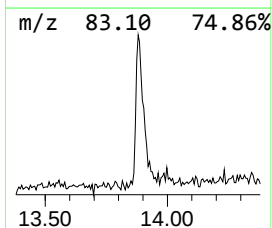
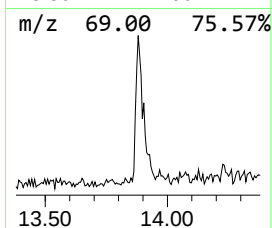
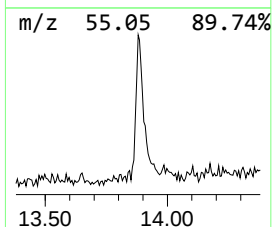
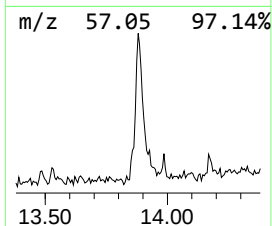
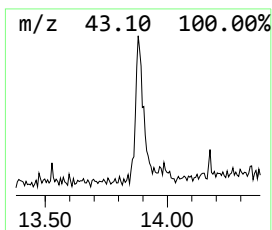
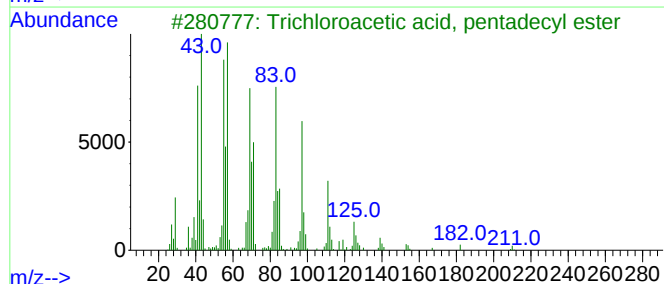
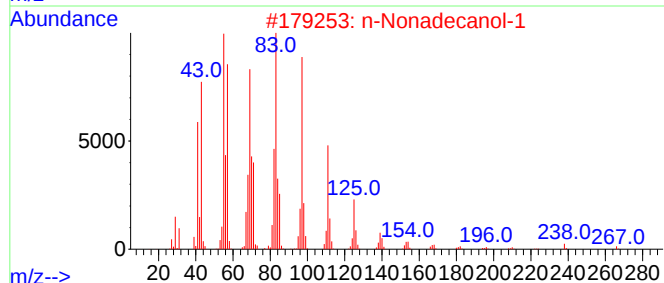
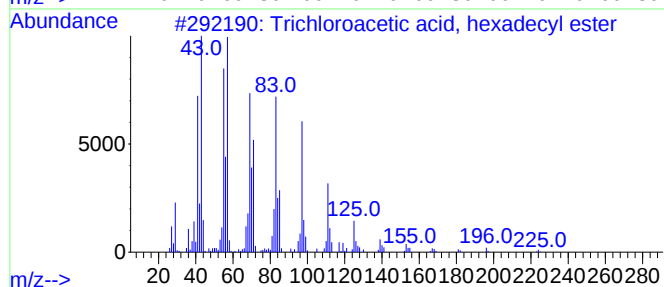
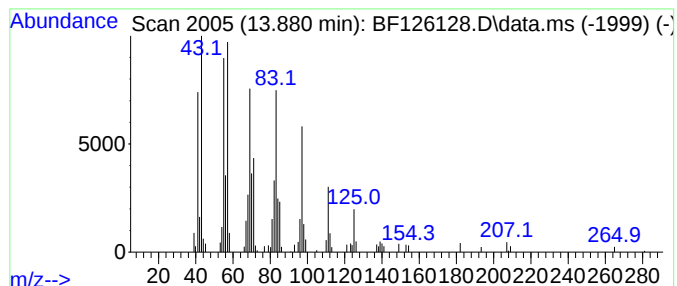
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Peak Number 2 Trichloroacetic acid, hexad... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.880	5.37 ng	309405	Chrysene-d12	14.004

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	95
2			n-Nonadecanol-1	284	C19H40O	001454-84-8	95
3			Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	94
4			Behenic alcohol	326	C22H46O	000661-19-8	91
5			1-Heneicosanol	312	C21H44O	015594-90-8	91



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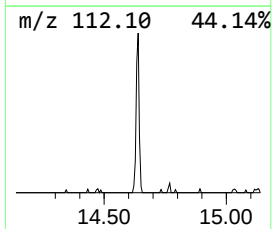
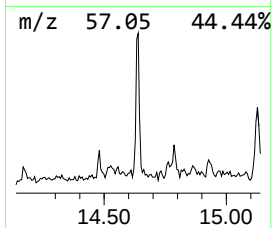
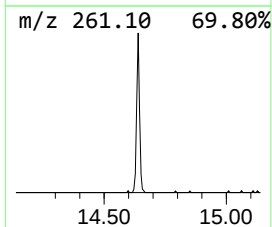
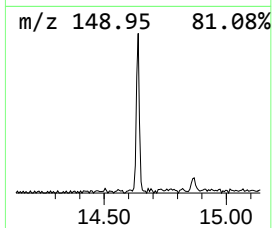
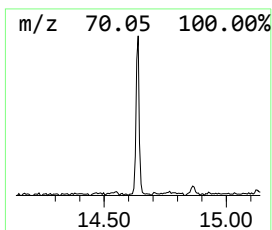
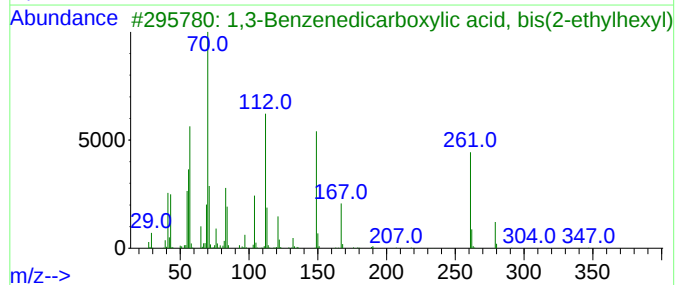
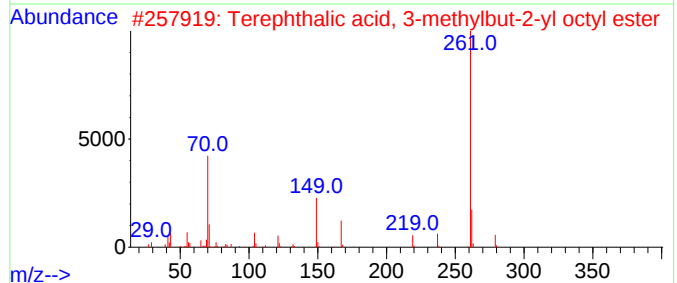
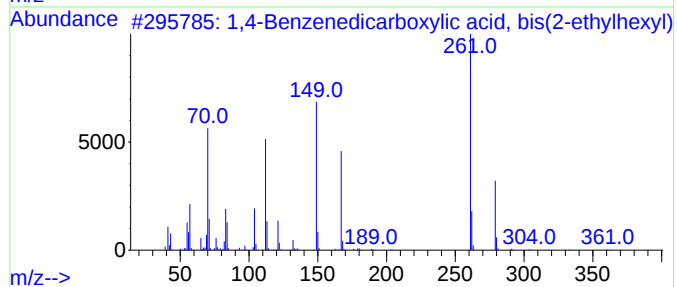
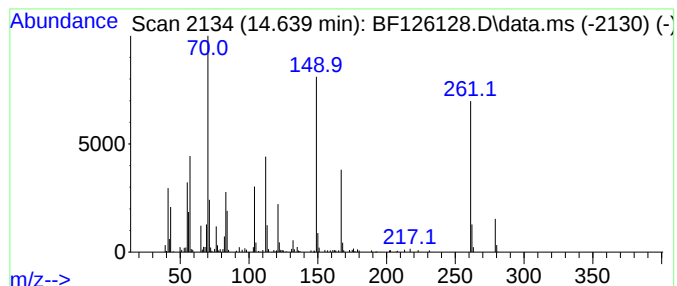
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Peak Number 3 1,4-Benzenedicarboxylic aci... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.639	5.17 ng	297986	Chrysene-d12	14.004

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,4-Benzenedicarboxylic acid, bi...	390	C24H38O4	006422-86-2	74
2			Terephthalic acid, 3-methylbut-2...	348	C21H32O4	1000356-27-6	59
3			1,3-Benzenedicarboxylic acid, bi...	390	C24H38O4	000137-89-3	52
4			Isophthalic acid, di(4-octyl) ester	390	C24H38O4	1000344-04-3	35
5			Terephthalic acid, di(4-octyl) e...	390	C24H38O4	1000323-74-2	27



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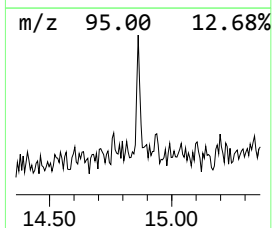
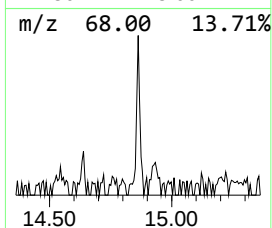
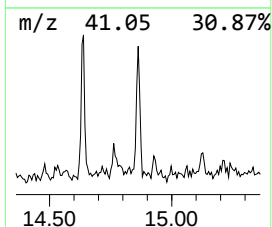
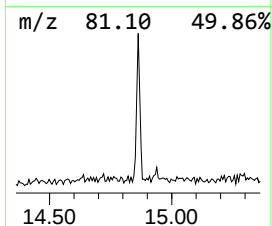
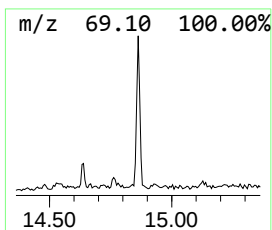
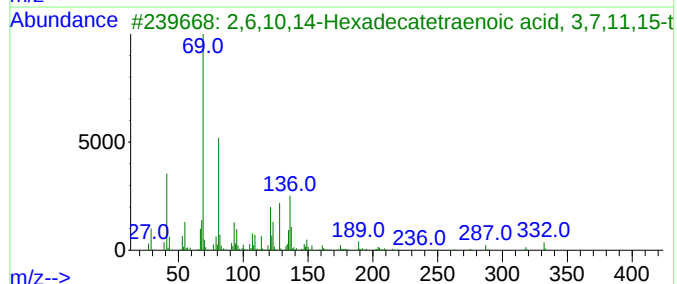
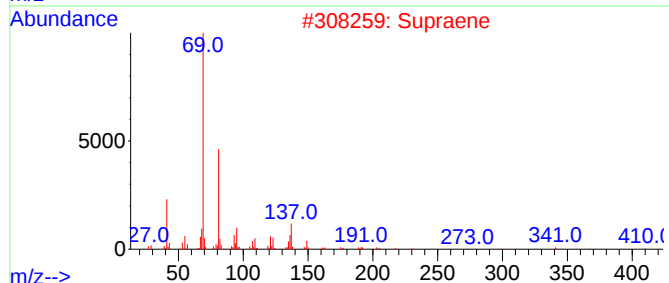
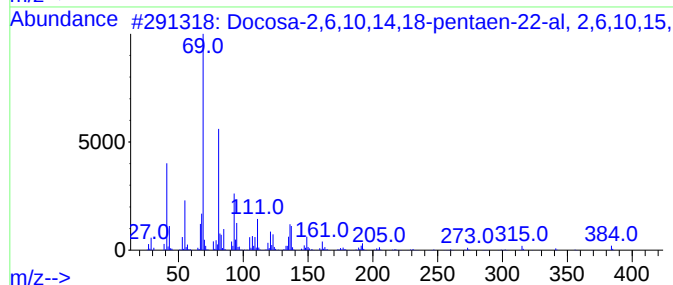
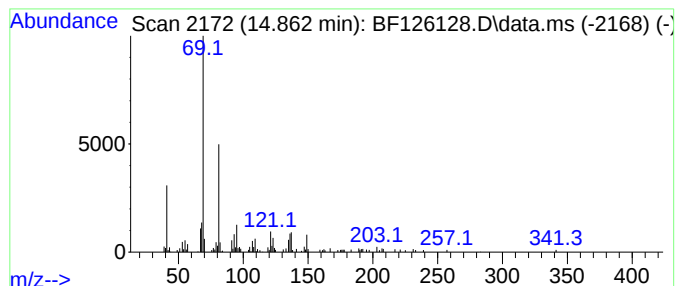
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Peak Number 4 Docosa-2,6,10,14,18-pentaen... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.862	2.69 ng	133570	Perylene-d12	15.468

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	90
2			Supraene	410	C30H50	007683-64-9	87
3			2,6,10,14-Hexadecatetraenoic aci...	332	C22H36O2	024035-35-6	72
4			4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	64
5			7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	64



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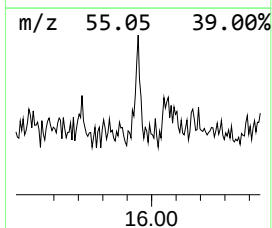
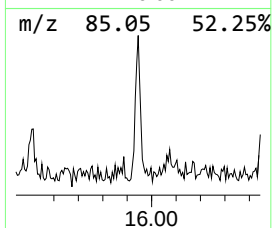
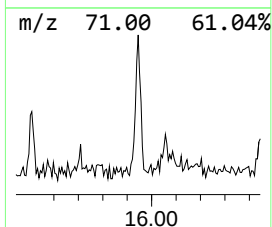
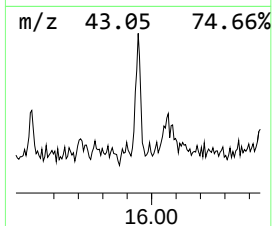
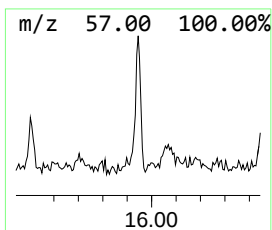
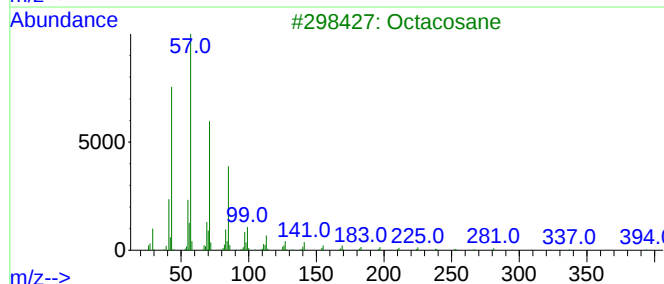
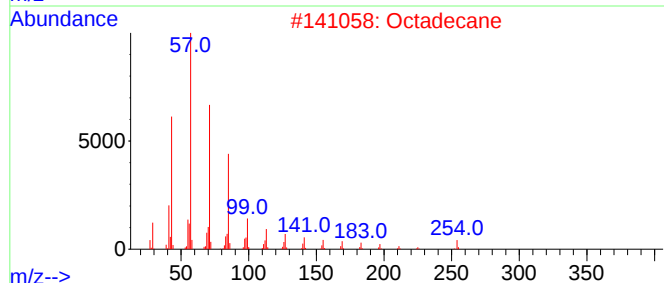
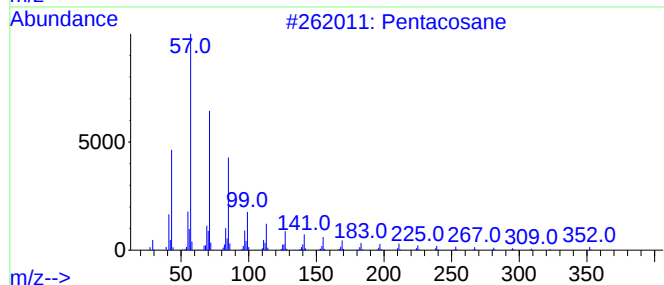
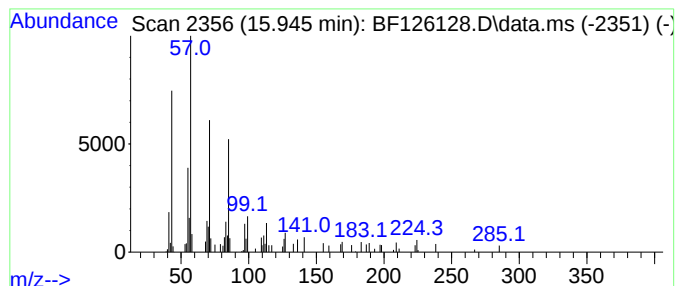
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Peak Number 5 Pentacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.945	2.10 ng	104363	Perylene-d12	15.468

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentacosane	352	C25H52	000629-99-2	87
2			Octadecane	254	C18H38	000593-45-3	87
3			Octacosane	394	C28H58	000630-02-4	87
4			Octacosane, 2-methyl-	408	C29H60	001560-98-1	87
5			Tetratetracontane	619	C44H90	007098-22-8	87



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Ethanol, 2-(2-b...	8.028	12.6	ng	702135	2	8.122	1113090	20.0
Trichloroacetic...	13.880	5.4	ng	309405	5	14.004	1152700	20.0
1,4-Benzenedica...	14.639	5.2	ng	297986	5	14.004	1152700	20.0
Docosa-2,6,10,1...	14.862	2.7	ng	133570	6	15.468	994304	20.0
Pentacosane	15.945	2.1	ng	104363	6	15.468	994304	20.0