

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF070722\
 Data File : BF129157.D
 Acq On : 07 Jul 2022 14:13
 Operator : CG\JU
 Sample : N3597-01
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 20220506-COMPOSITE-A

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-BF062922.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF129157.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.198	492	495	502	rVB	51724	66890	1.14%	0.141%
2	5.575	554	559	562	rBV	6052155	5783620	98.63%	12.221%
3	6.575	723	729	731	rBV	5372660	5863898	100.00%	12.391%
4	6.592	731	732	741	rVB	259790	233719	3.99%	0.494%
5	6.951	789	793	796	rBV	2123959	1667375	28.43%	3.523%
6	7.510	883	888	892	rBV	3632020	3607283	61.52%	7.623%
7	8.234	1007	1011	1015	rBV	2670165	2226021	37.96%	4.704%
8	9.310	1189	1194	1197	rBV	6690552	5598665	95.48%	11.831%
9	9.992	1306	1310	1314	rBV	2704279	2344064	39.97%	4.953%
10	10.786	1440	1445	1448	rBV	5191431	4604776	78.53%	9.730%
11	11.486	1560	1564	1568	rBV	3146137	2605833	44.44%	5.506%
12	11.551	1572	1575	1578	rBV3	104223	86304	1.47%	0.182%
13	11.998	1645	1651	1661	rBV2	584904	748762	12.77%	1.582%
14	12.704	1767	1771	1776	rBV	85039	92144	1.57%	0.195%
15	12.786	1780	1785	1795	rBV	162377	228456	3.90%	0.483%
16	12.933	1805	1810	1813	rBV	71479	76035	1.30%	0.161%
17	13.074	1830	1834	1838	rBV	6053426	5758632	98.20%	12.169%
18	13.963	1982	1985	1988	rVB	68967	65535	1.12%	0.138%
19	14.057	1993	2001	2005	rBV4	93367	287391	4.90%	0.607%
20	14.104	2006	2009	2011	rVB	83219	83272	1.42%	0.176%
21	14.139	2011	2015	2018	rBV	2734304	2320215	39.57%	4.903%
22	14.227	2025	2030	2036	rBV	455470	468318	7.99%	0.990%
23	14.280	2036	2039	2045	rVB	63472	68274	1.16%	0.144%
24	14.586	2088	2091	2095	rVB	67092	66740	1.14%	0.141%
25	14.992	2156	2160	2164	rBV	459349	461731	7.87%	0.976%
26	15.263	2203	2206	2212	rVB	59896	74566	1.27%	0.158%
27	15.662	2268	2274	2282	rBV	1465521	1834854	31.29%	3.877%

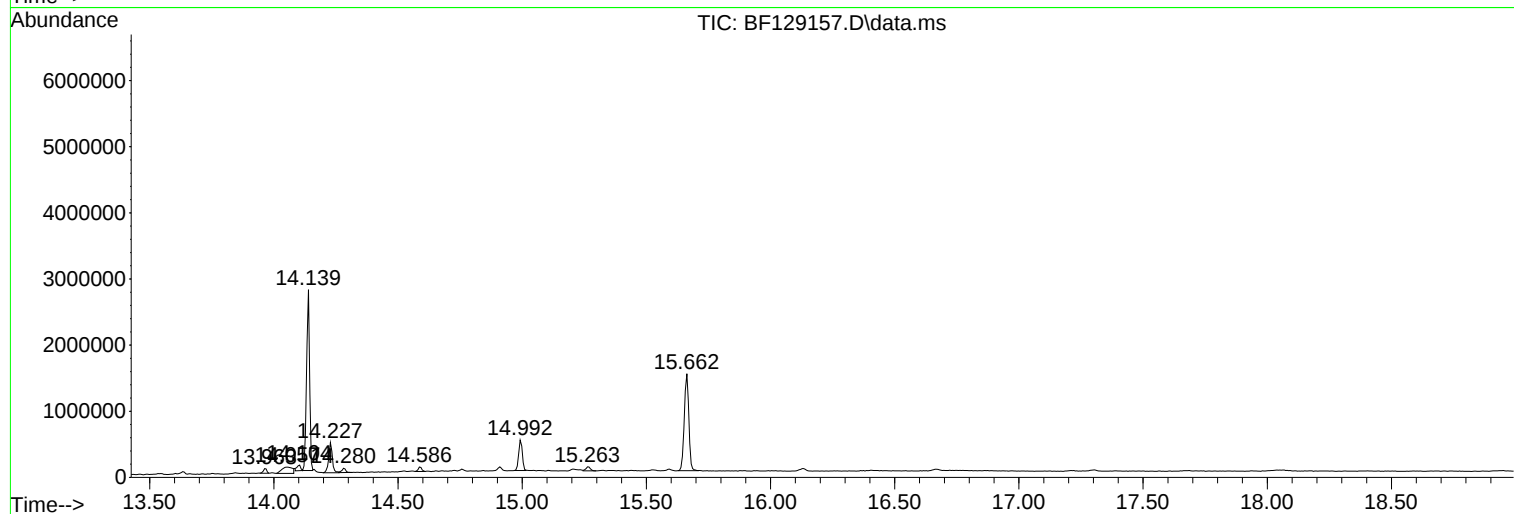
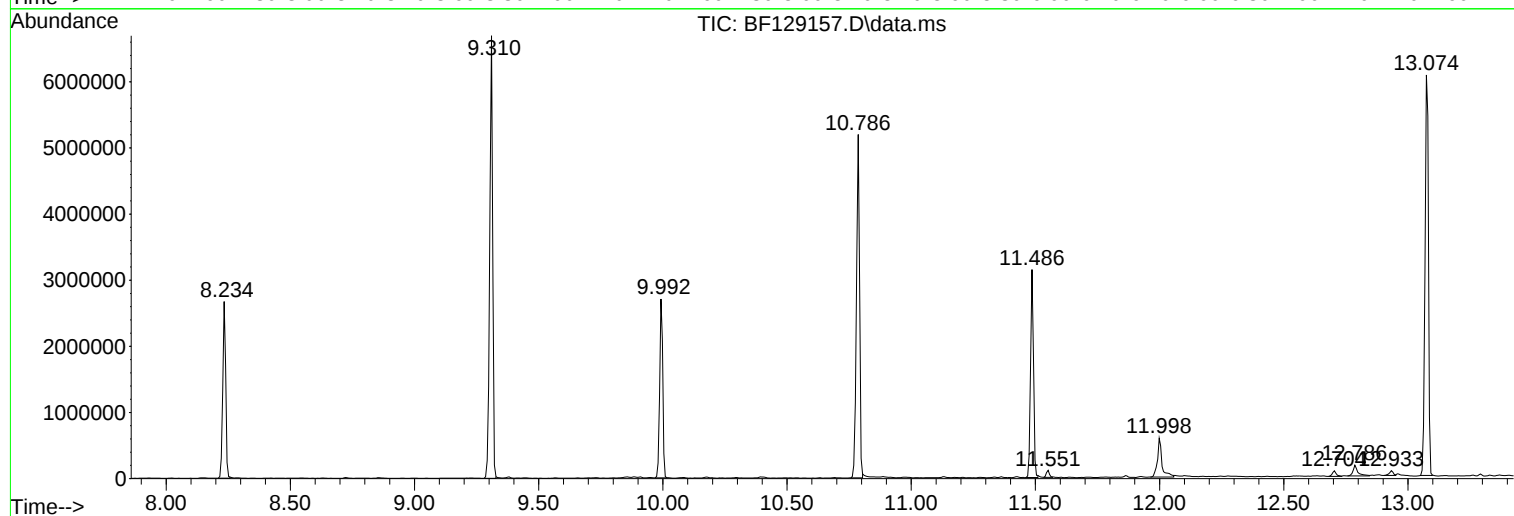
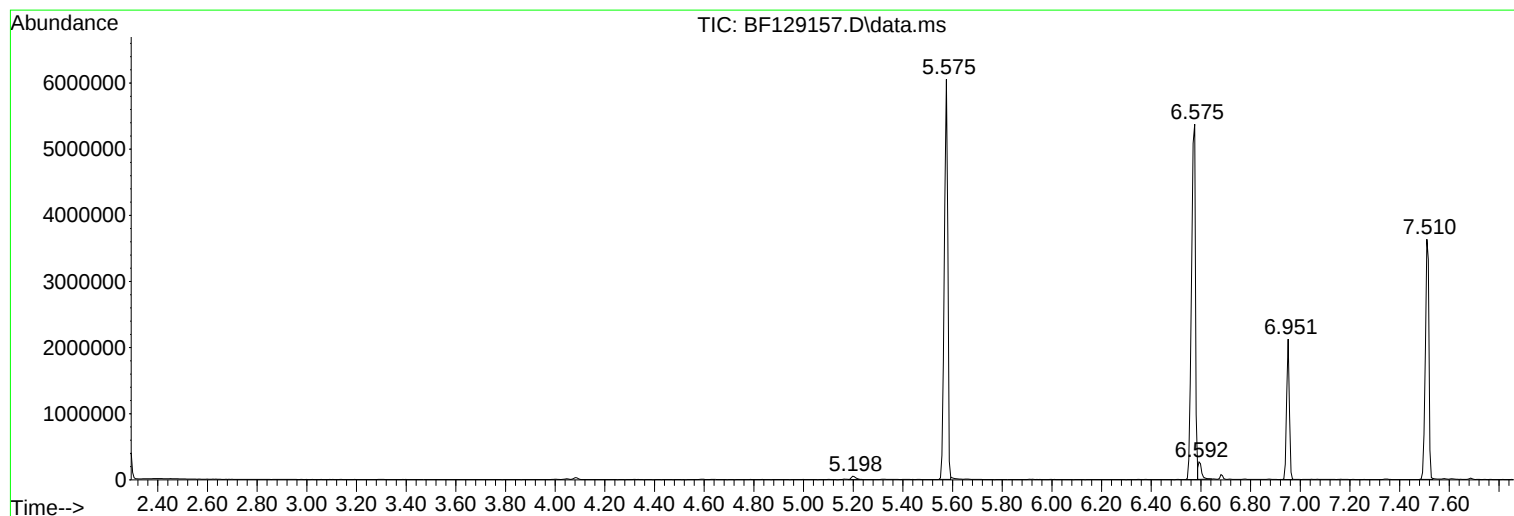
Sum of corrected areas: 47323373

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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062922.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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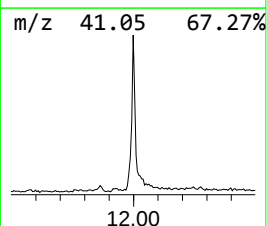
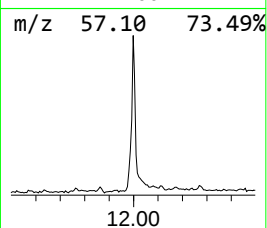
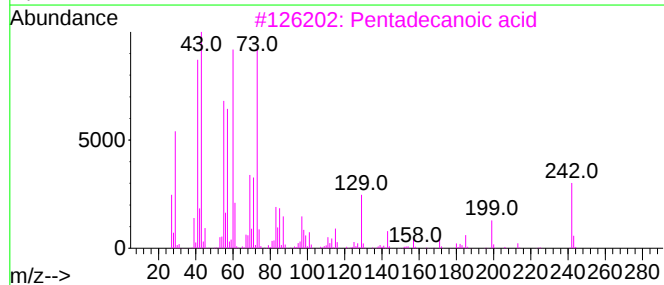
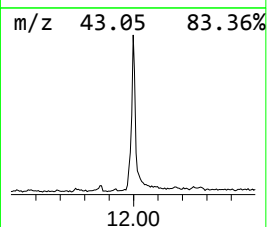
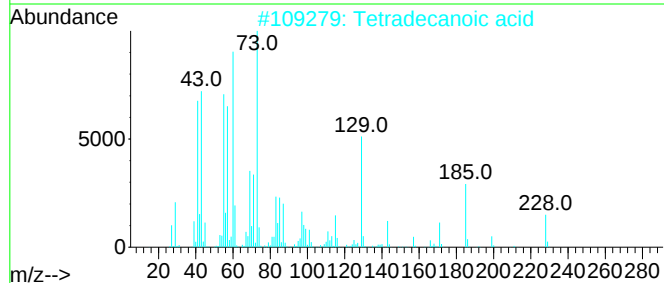
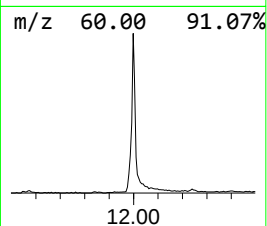
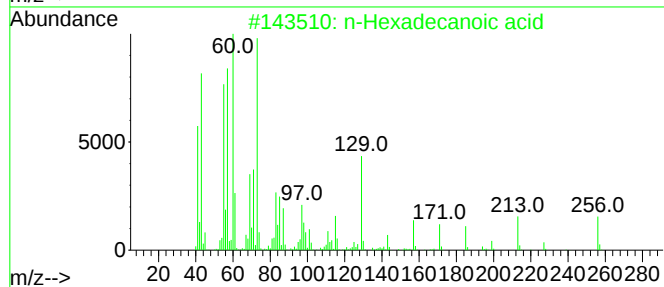
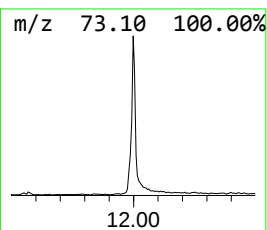
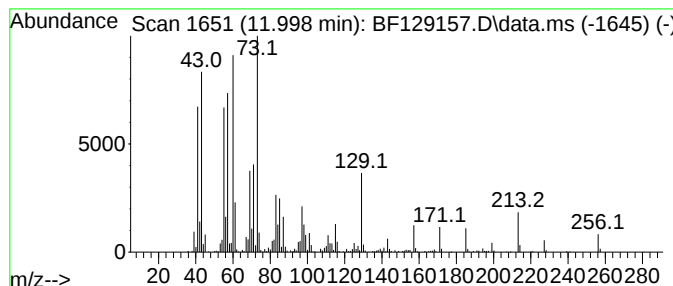
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.998	5.75 ng	748762	Phenanthrene-d10	11.486

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	93
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	86
4			Tridecanoic acid	214	C13H26O2	000638-53-9	76
5			Nonanoic acid	158	C9H18O2	000112-05-0	43



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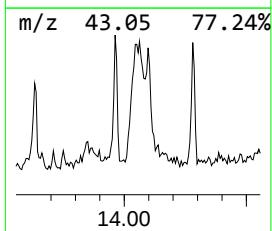
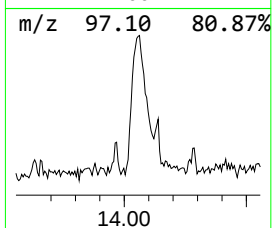
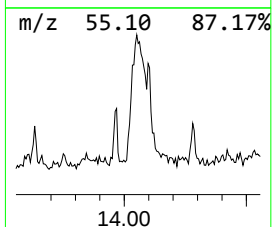
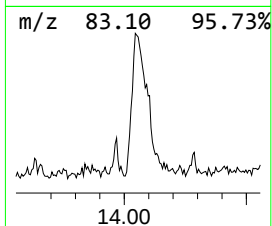
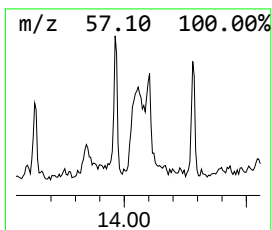
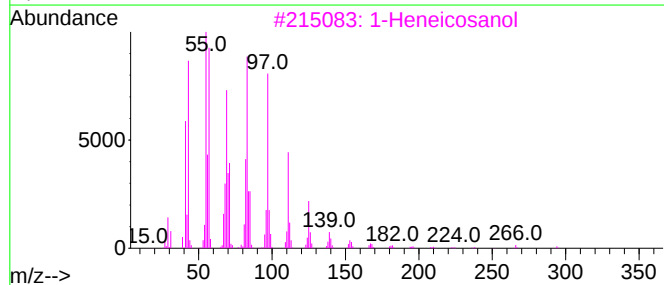
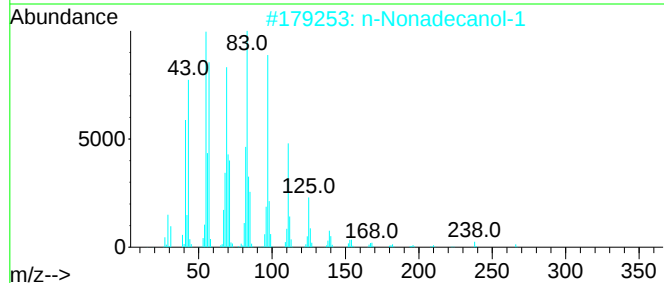
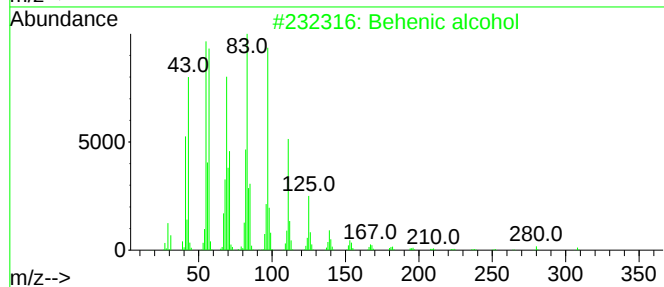
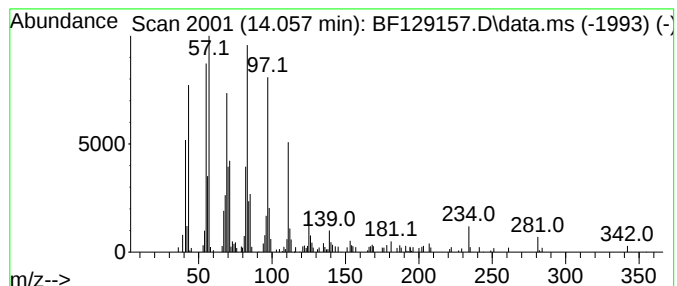
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Behenic alcohol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.057	2.48 ng	287391	Chrysene-d12	14.139

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Behenic alcohol	326	C22H46O	000661-19-8	95
2		n-Nonadecanol-1	284	C19H40O	001454-84-8	95
3		1-Heneicosanol	312	C21H44O	015594-90-8	95
4		1-Tricosene	322	C23H46	018835-32-0	93
5		n-Heptadecanol-1	256	C17H36O	001454-85-9	90



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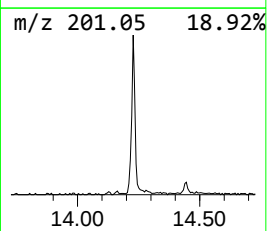
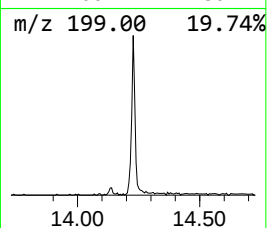
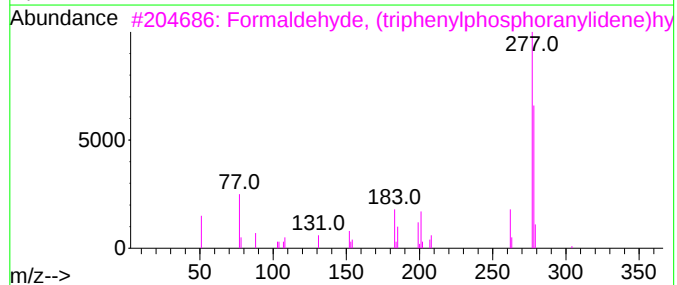
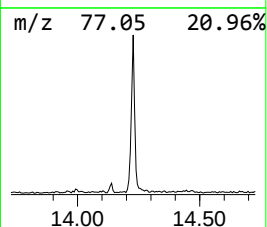
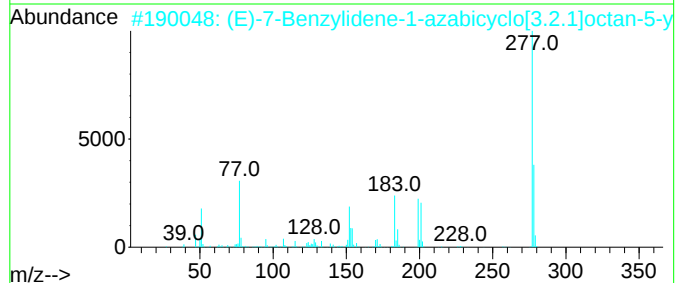
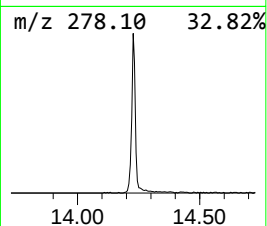
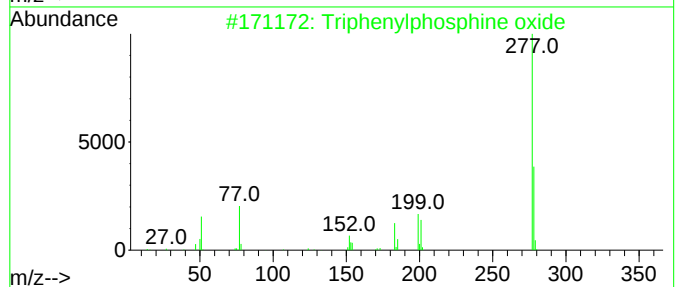
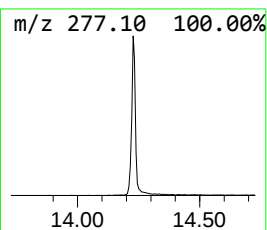
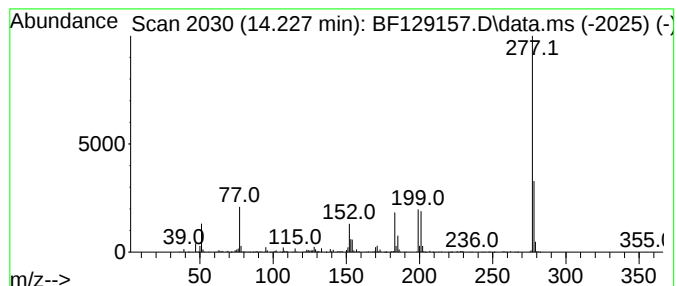
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Peak Number 3 Triphenylphosphine oxide Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.227	4.04 ng	468318	Chrysene-d12	14.139

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triphenylphosphine oxide	278	C18H15OP	000791-28-6	97
2			(E)-7-Benzylidene-1-azabicyclo[3...]	293	C15H19NO3S	1000483-83-4	91
3			Formaldehyde, (triphenylphosphor...]	304	C19H17N2P	015990-54-2	59
4			Cobalt,(.eta.<5>-2,4-cyclopentad...	277	C16H15BCo	036682-12-9	38
5			3-(3,4-Dichlorophenyl)-2-thioxo-...	277	C9H5Cl2NOS2	017046-34-3	32



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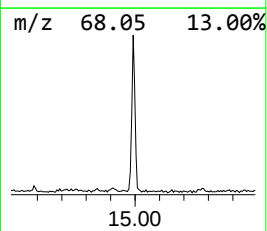
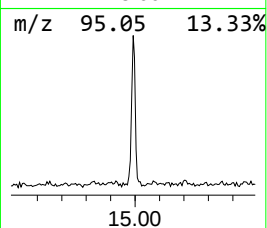
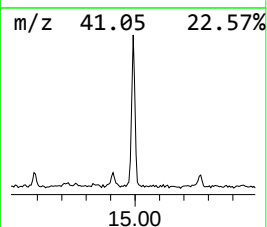
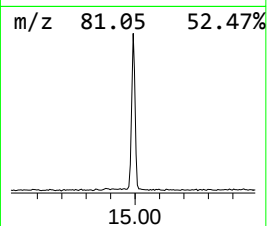
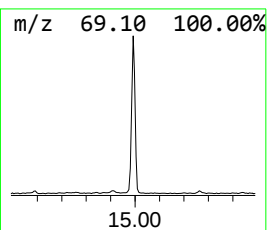
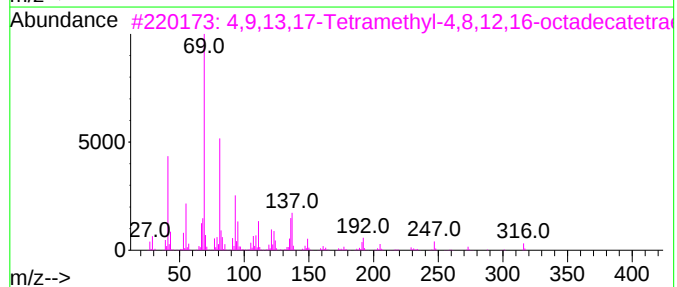
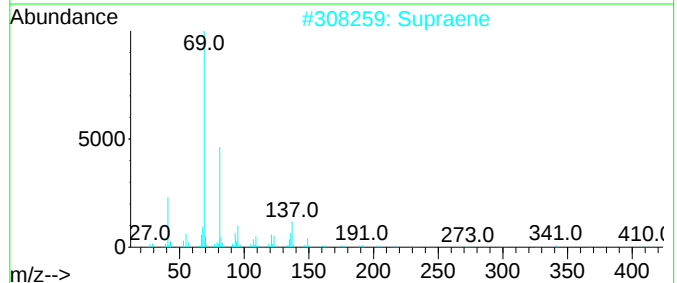
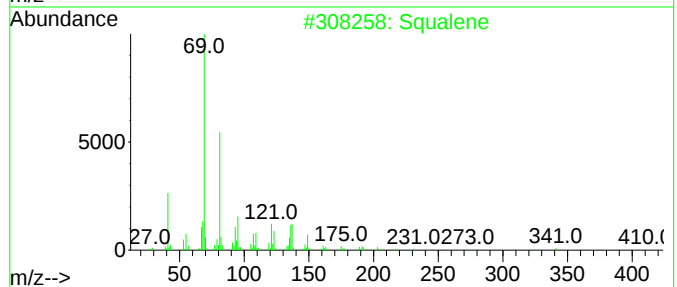
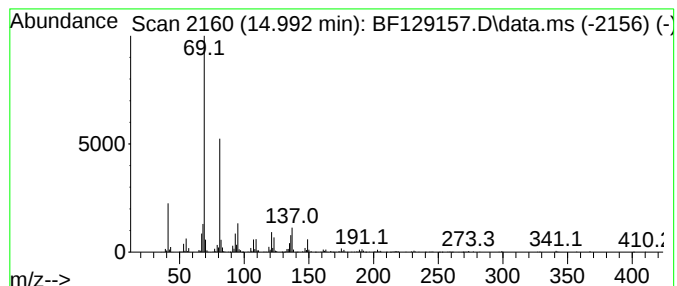
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Peak Number 4 Squalene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.992	5.03 ng	461731	Perylene-d12	15.663

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Squalene	410	C30H50	000111-02-4	95
2			Supraene	410	C30H50	007683-64-9	91
3			4,9,13,17-Tetramethyl-4,8,12,16-...	316	C22H36O	056882-09-8	83
4			2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	004602-84-0	72
5			2,3,5-Trimethyl-2,3,5-hexanetric...	203	C12H17N3	003974-79-6	50



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
n-Hexadecanoic ...	11.998	5.8	ng	748762	4	11.486	2605830	20.0
Behenic alcohol	14.057	2.5	ng	287391	5	14.139	2320220	20.0
Triphenylphosph...	14.227	4.0	ng	468318	5	14.139	2320220	20.0
Squalene	14.992	5.0	ng	461731	6	15.663	1834850	20.0