

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010622\
 Data File : BF126530.D
 Acq On : 6 Jan 2022 20:43
 Operator : JU/CG
 Sample : M5196-05
 Misc :
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 COMPOSITE-SAMPLE-3-SHALLOW

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-BF122921.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF126530.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.140	5	9	18	rVB	32059	44300	2.40%	0.349%
2	4.987	489	493	502	rVB	55756	76861	4.17%	0.606%
3	5.392	558	562	565	rBV	1954049	1839000	99.78%	14.506%
4	6.410	730	735	738	rBV	1823847	1842976	100.00%	14.537%
5	6.781	794	798	801	rBV	536742	450431	24.44%	3.553%
6	7.339	888	893	896	rBV	1322342	1180786	64.07%	9.314%
7	8.063	1012	1016	1019	rBV	684224	578589	31.39%	4.564%
8	9.139	1194	1199	1202	rBV	1982990	1688626	91.62%	13.319%
9	9.227	1210	1214	1219	rVB	23515	22142	1.20%	0.175%
10	9.816	1310	1314	1318	rBV	663129	523802	28.42%	4.132%
11	10.604	1444	1448	1452	rBV	917967	776638	42.14%	6.126%
12	10.710	1462	1466	1470	rBV2	19275	25805	1.40%	0.204%
13	11.304	1563	1567	1570	rBV	483069	422848	22.94%	3.335%
14	11.839	1655	1658	1667	rBV2	92823	99443	5.40%	0.784%
15	12.627	1789	1792	1799	rBV2	31283	41127	2.23%	0.324%
16	12.892	1833	1837	1840	rBV	1481181	1274588	69.16%	10.054%
17	13.798	1987	1991	2005	rBV	146708	274223	14.88%	2.163%
18	13.945	2012	2016	2020	rBV	545060	463991	25.18%	3.660%
19	14.045	2030	2033	2037	rBV	47861	49238	2.67%	0.388%
20	14.427	2095	2098	2101	rBV	23159	28215	1.53%	0.223%
21	14.709	2142	2146	2153	rBV	334612	378231	20.52%	2.983%
22	15.062	2203	2206	2210	rVB	30039	35012	1.90%	0.276%
23	15.392	2257	2262	2266	rBV2	424627	494340	26.82%	3.899%
24	15.433	2266	2269	2275	rVB4	20367	26317	1.43%	0.208%
25	15.862	2338	2342	2346	rVB2	30615	40419	2.19%	0.319%

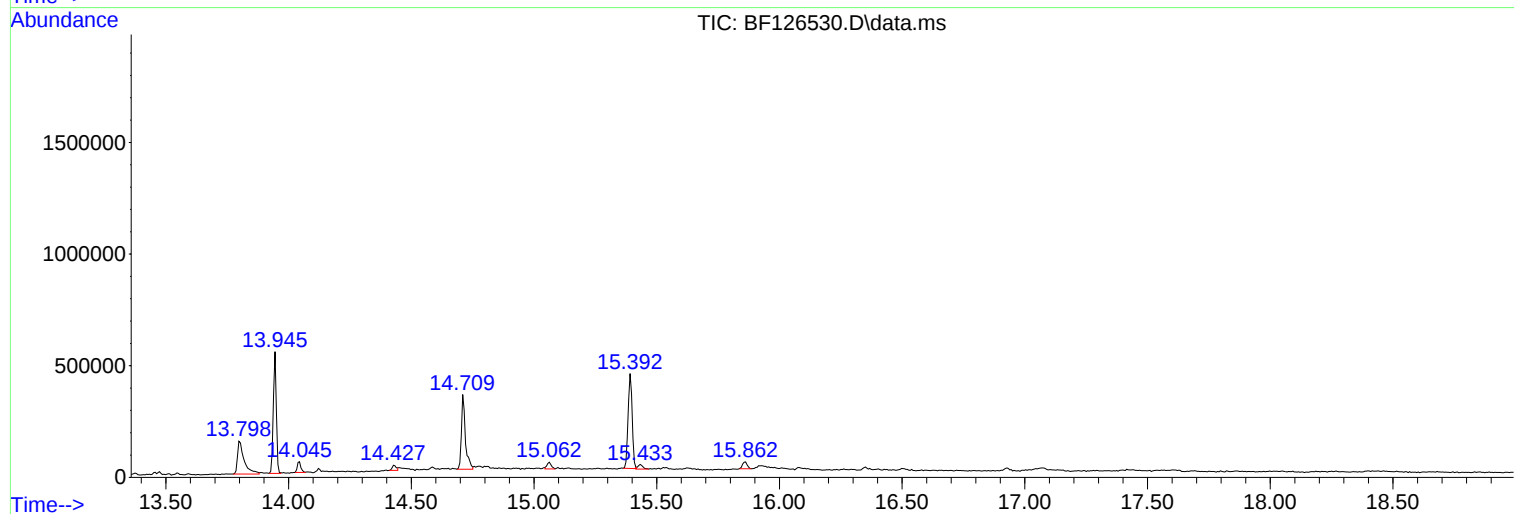
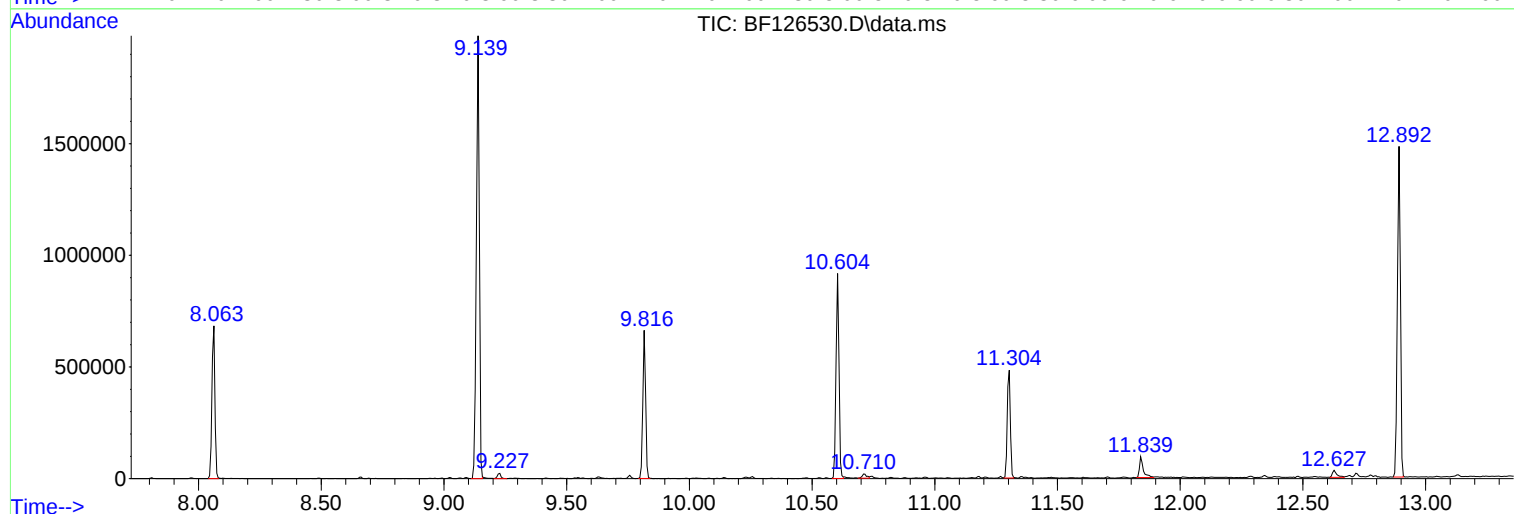
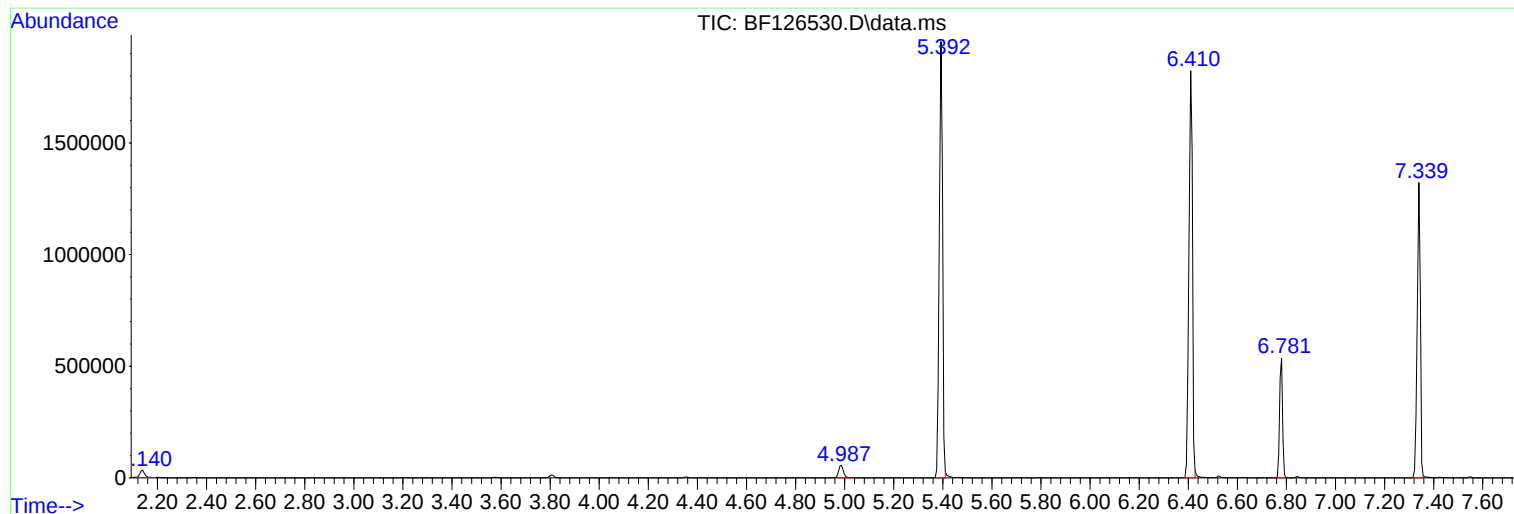
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ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMPOSITE-SAMPLE-3-SHALLOW

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122921.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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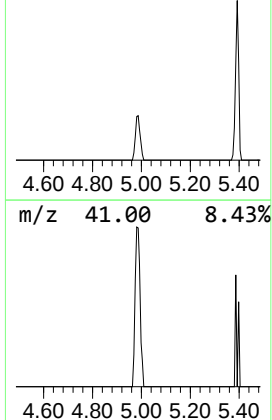
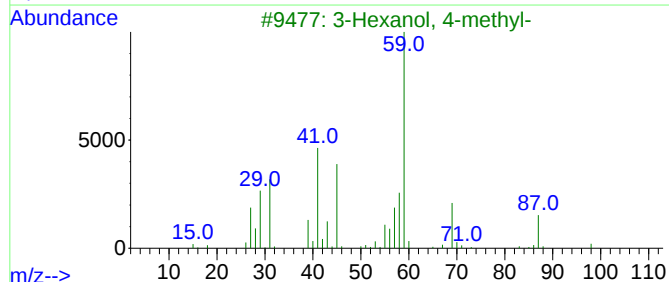
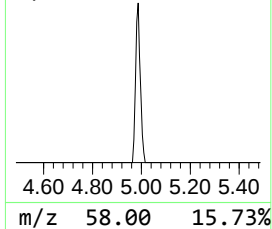
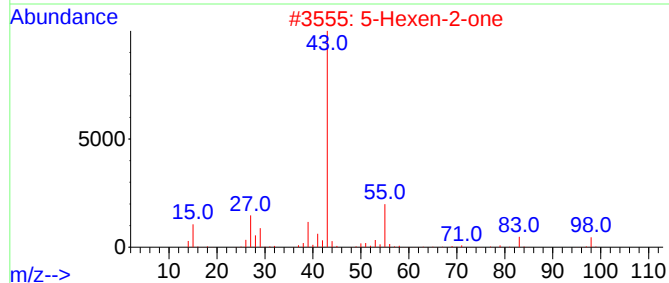
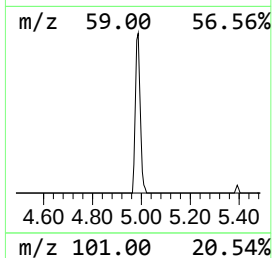
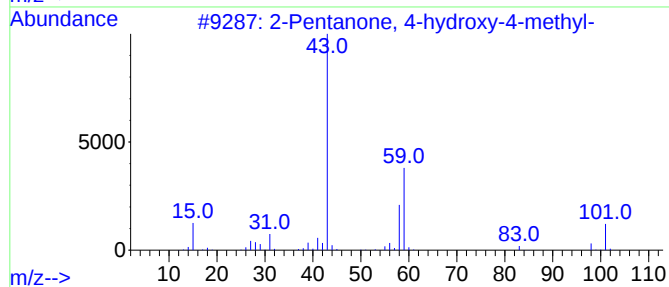
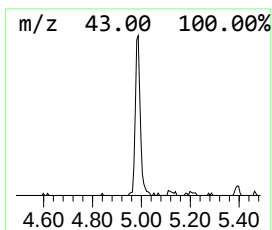
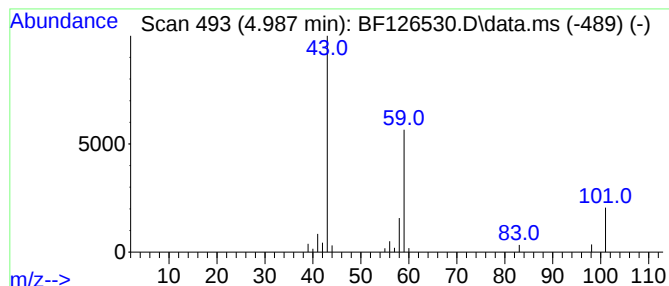
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Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.987	3.41 ng	76861	1,4-Dichlorobenzene-d4	6.781

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		5-Hexen-2-one	98	C6H10O	000109-49-9	9
3		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	9
4		3-Octanol	130	C8H18O	000589-98-0	9
5		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	9



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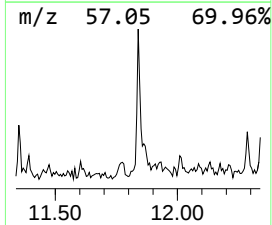
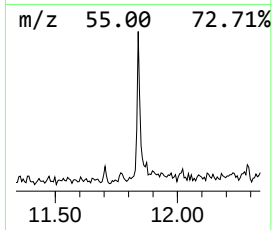
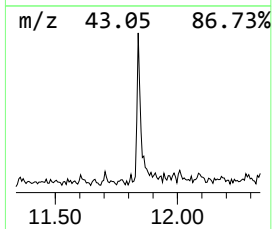
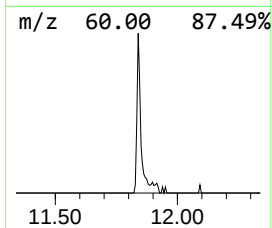
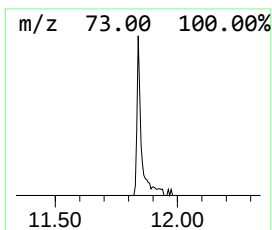
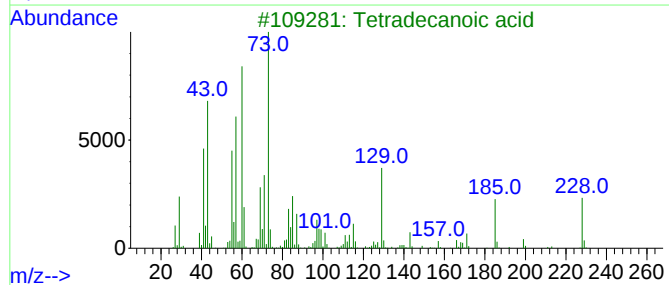
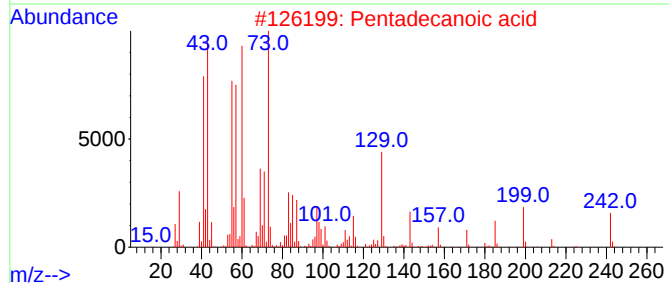
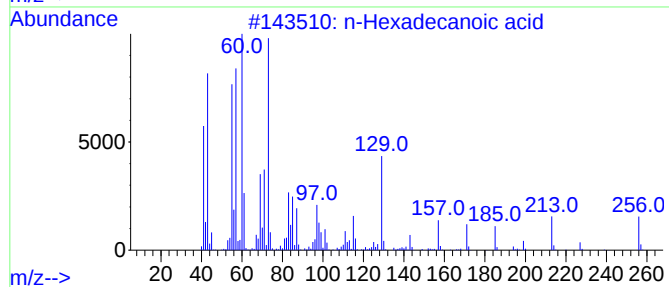
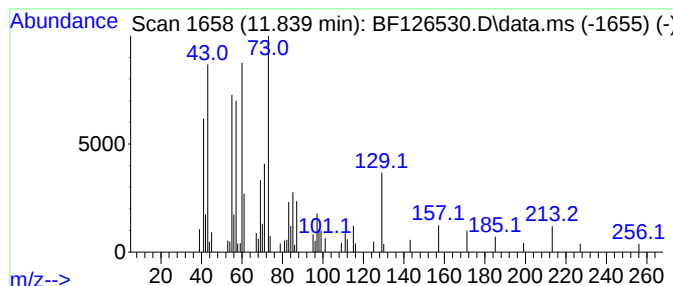
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Peak Number 2 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.839	4.70 ng	99443	Phenanthrene-d10	11.304

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	87
4			Carbonic acid, decyl tridecyl ester	384	C24H48O3	1000383-16-2	11
5			1-Octadecanesulphonyl chloride	352	C18H37ClO2S	1000342-70-4	11



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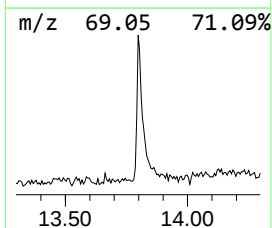
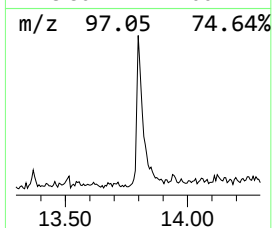
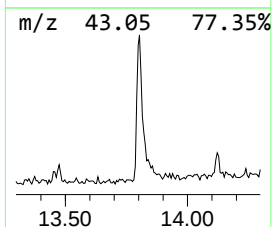
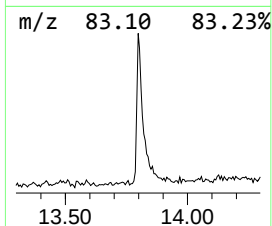
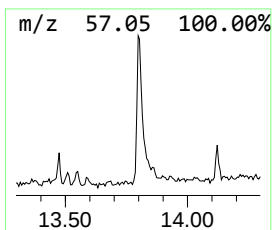
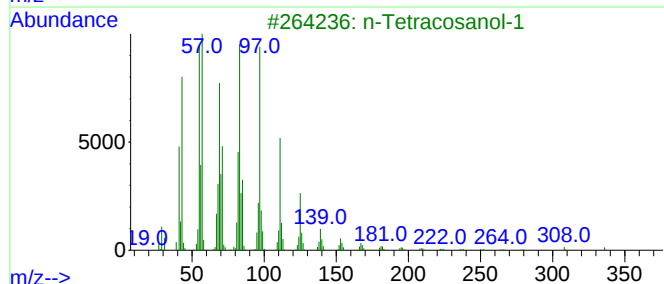
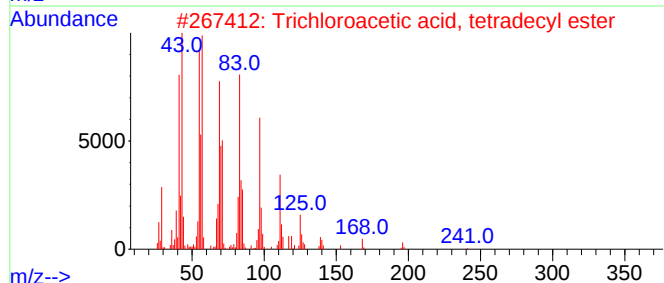
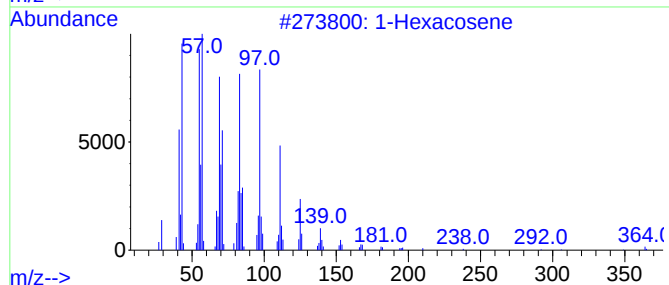
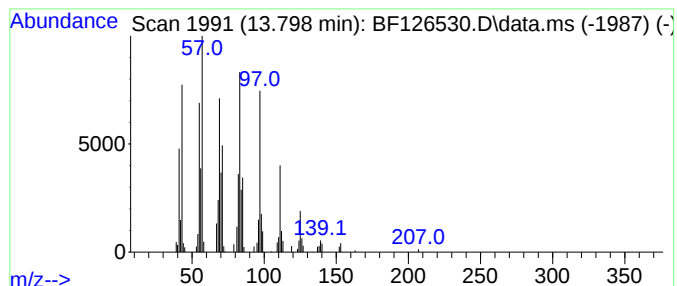
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Peak Number 3 1-Hexacosene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.798	11.82 ng	274223	Chrysene-d12	13.945

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexacosene			364	C26H52	018835-33-1	94
2	Trichloroacetic acid, tetradecyl...			358	C16H29Cl3O2	074339-52-9	91
3	n-Tetracosanol-1			354	C24H50O	000506-51-4	91
4	Trichloroacetic acid, hexadecyl ...			386	C18H33Cl3O2	074339-54-1	91
5	1-Heptacosanol			396	C27H56O	002004-39-9	91



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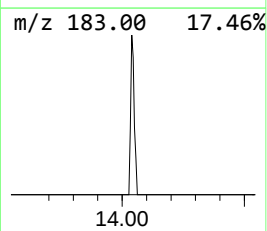
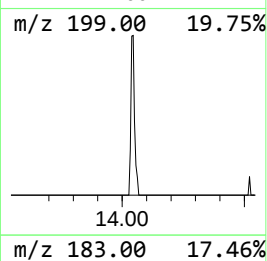
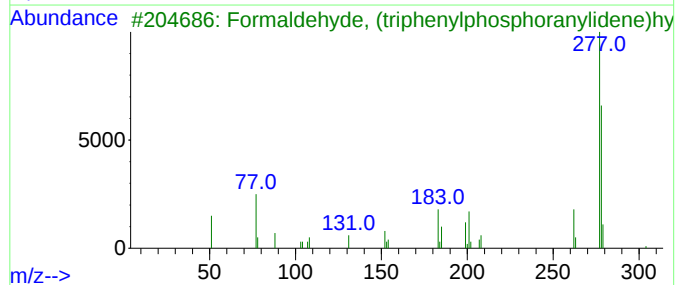
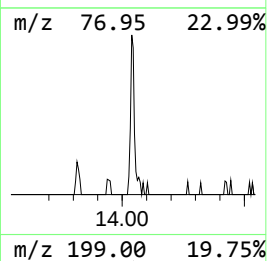
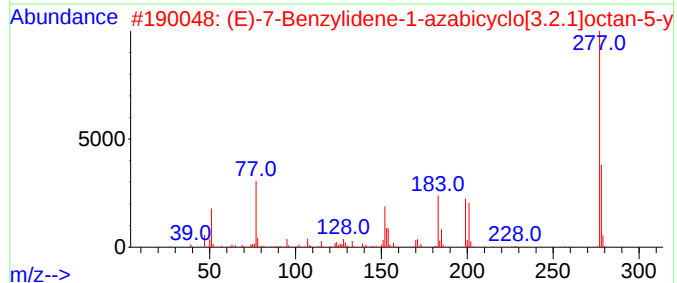
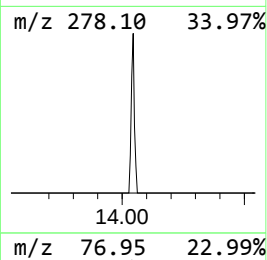
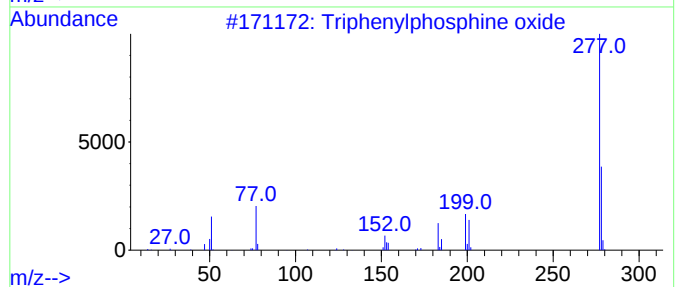
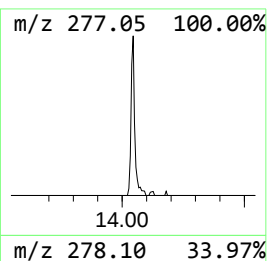
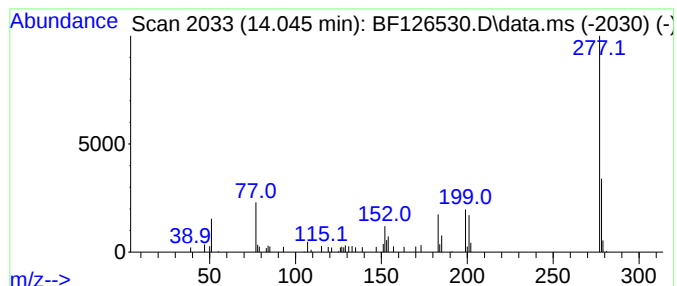
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Triphenylphosphine oxide Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.045	2.12 ng	49238	Chrysene-d12	13.945

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	90
3			Formaldehyde, (triphenylphosphor...]	304	C19H17N2P	015990-54-2	50
4			Vanadium, cycloheptatrienyl-(pen...]	277	C17H22V	1000155-20-5	49
5			Cobalt, (.eta.<5>-2,4-cyclopentad...]	277	C16H15BCo	036682-12-9	28



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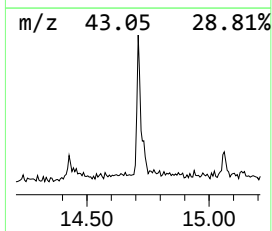
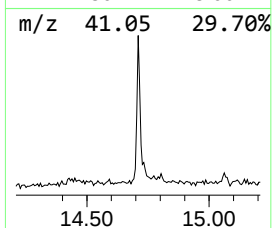
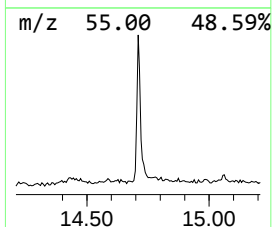
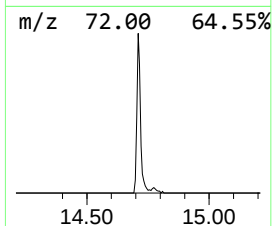
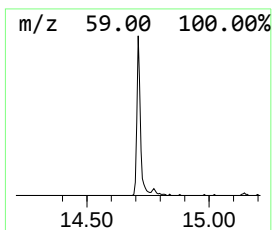
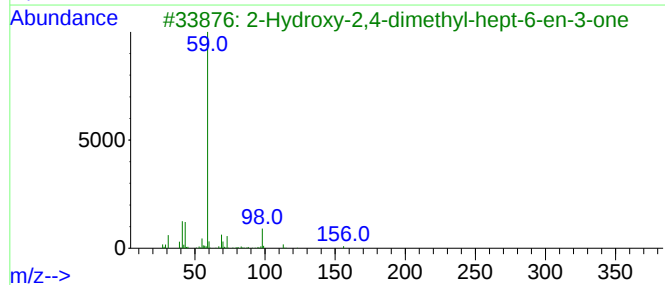
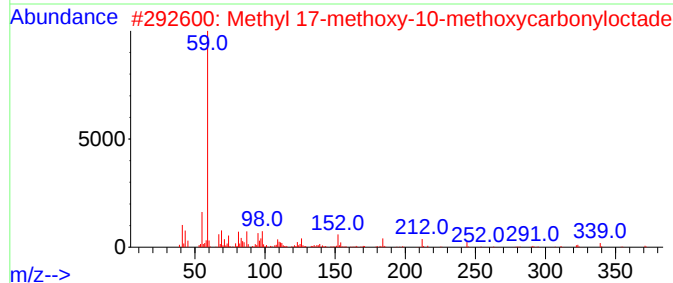
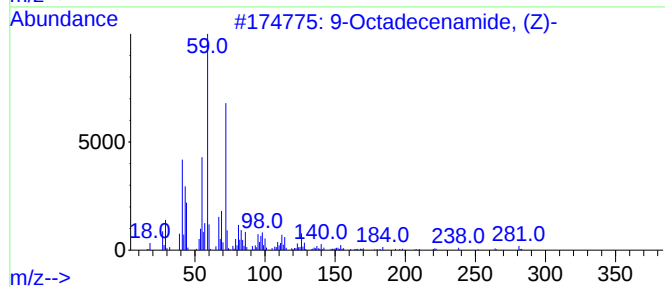
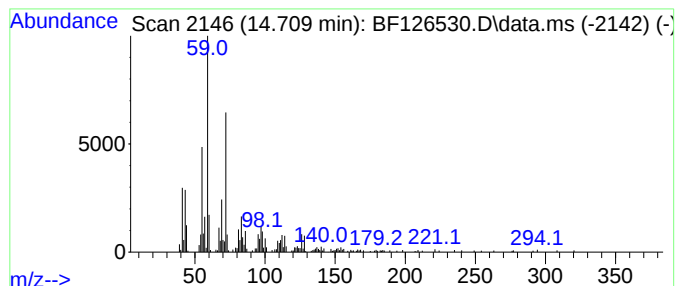
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 9-Octadecenamide, (Z)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.709	15.30 ng	378231	Perylene-d12	15.392	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	90
2	Methyl 17-methoxy-10-methoxycarb...	386	C22H42O5	1000110-20-7	43
3	2-Hydroxy-2,4-dimethyl-hept-6-en...	156	C9H16O2	1000192-56-0	43
4	1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	38
5	4-Ethyl-3-octanol	158	C10H22O	019781-26-1	38



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	4.987	3.4	ng	76861	1	6.781	450431	20.0
n-Hexadecanoic ...	11.839	4.7	ng	99443	4	11.304	422848	20.0
1-Hexacosene	13.798	11.8	ng	274223	5	13.945	463991	20.0
Triphenylphosph...	14.045	2.1	ng	49238	5	13.945	463991	20.0
9-Octadecenamid...	14.709	15.3	ng	378231	6	15.392	494340	20.0