

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060821\
 Data File : BF124179.D
 Acq On : 8 Jun 2021 14:25
 Operator : JU/CG
 Sample : M2613-03
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 18-B12(94-98)

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-BF060321.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF124179.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.134	3	8	13	rVB	607823	791223	44.76%	7.232%
2	5.492	575	579	582	rBV	1464669	1322188	74.80%	12.084%
3	6.504	746	751	754	rBV	1312490	1297032	73.37%	11.854%
4	6.857	808	811	814	rBV	314290	229612	12.99%	2.099%
5	7.422	902	907	910	rBV	909238	895697	50.67%	8.186%
6	8.139	1025	1029	1033	rBV	343509	279442	15.81%	2.554%
7	9.222	1208	1213	1216	rBV	1846097	1574330	89.06%	14.389%
8	9.898	1324	1328	1331	rBV	445446	341596	19.32%	3.122%
9	10.692	1458	1463	1466	rBV	1541251	1282679	72.56%	11.723%
10	11.386	1577	1581	1584	rBV	447183	364594	20.63%	3.332%
11	11.910	1667	1670	1673	rBV2	54180	42970	2.43%	0.393%
12	12.974	1846	1851	1854	rBV	2019815	1767714	100.00%	16.156%
13	13.892	2001	2007	2023	rBV6	34879	112840	6.38%	1.031%
14	14.027	2027	2030	2034	rVB	370339	340374	19.26%	3.111%
15	14.880	2171	2175	2178	rBV	32677	32398	1.83%	0.296%
16	15.509	2276	2282	2287	rBV2	206316	266641	15.08%	2.437%

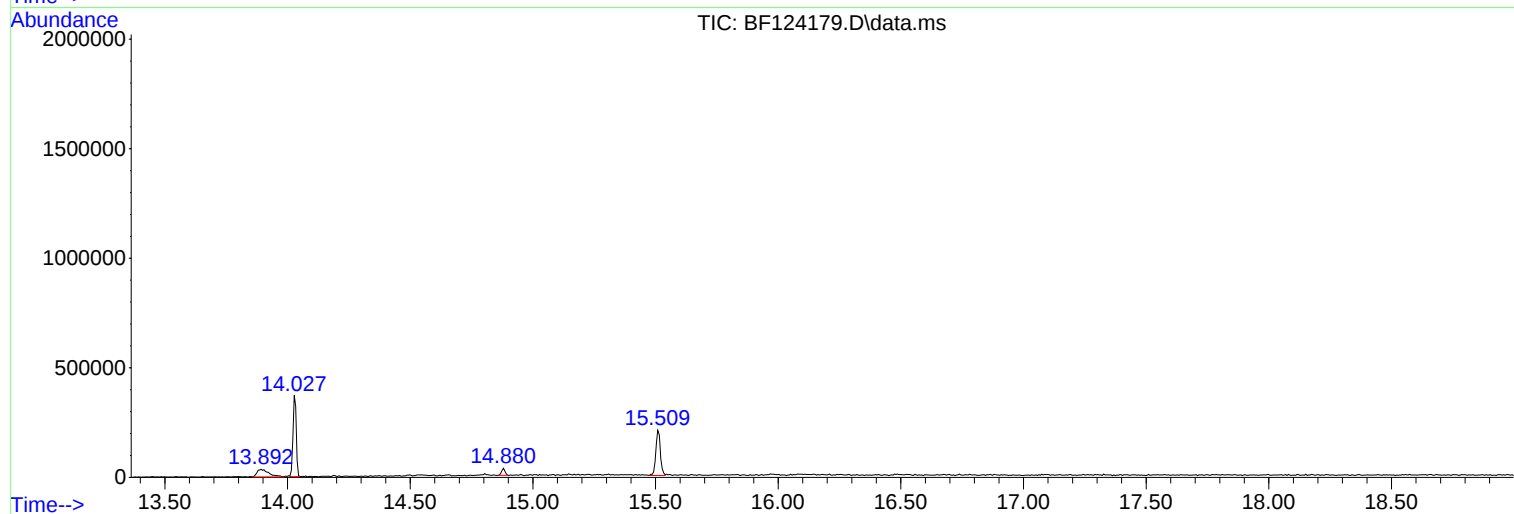
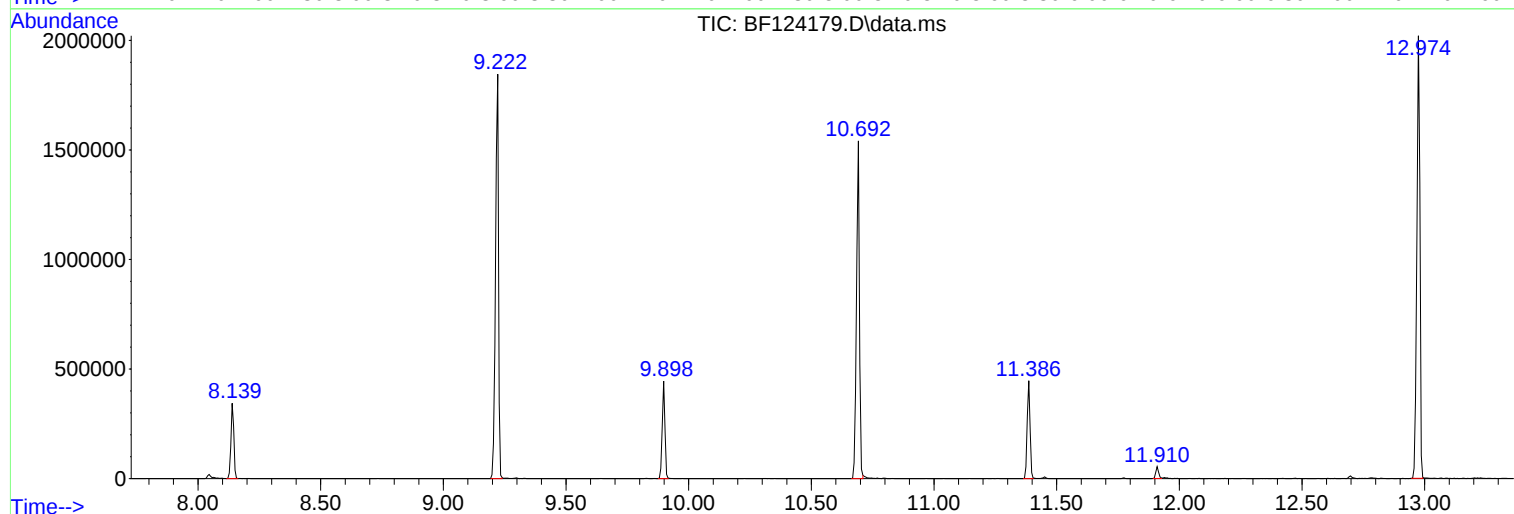
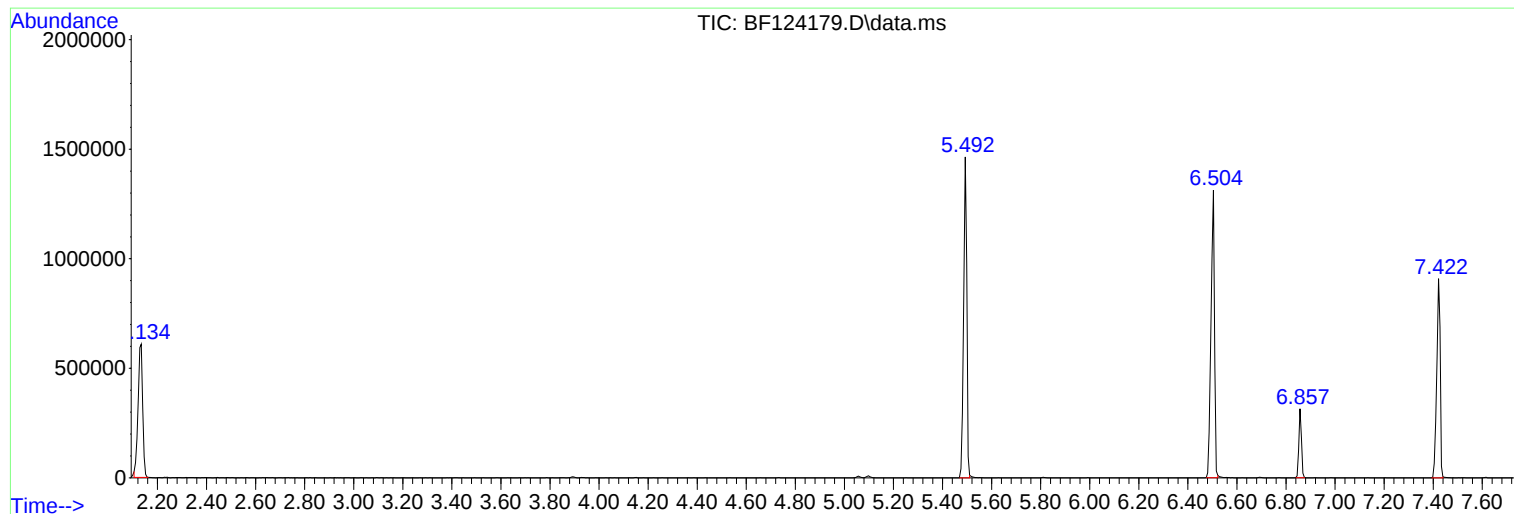
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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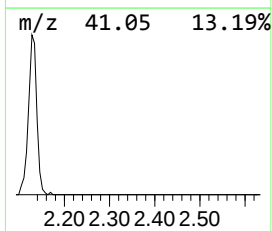
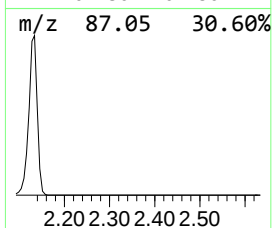
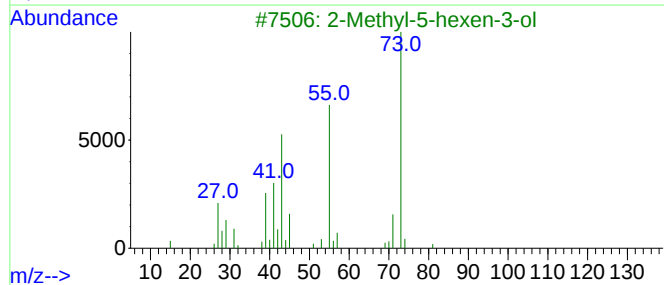
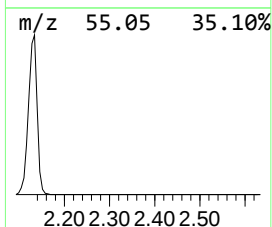
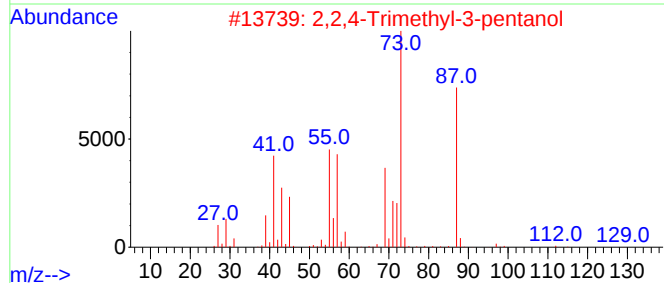
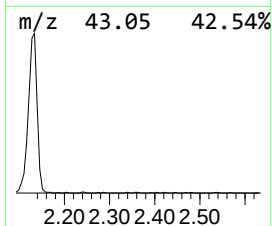
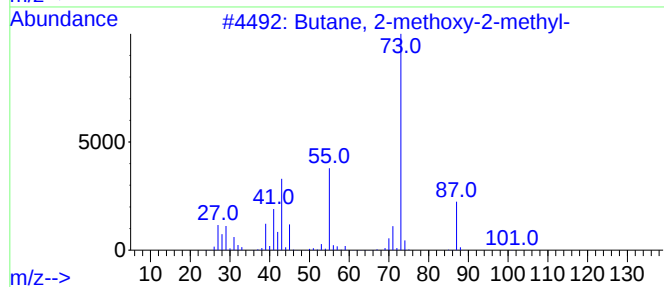
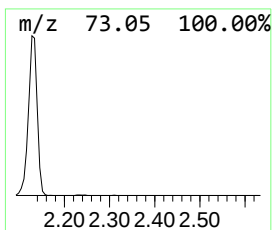
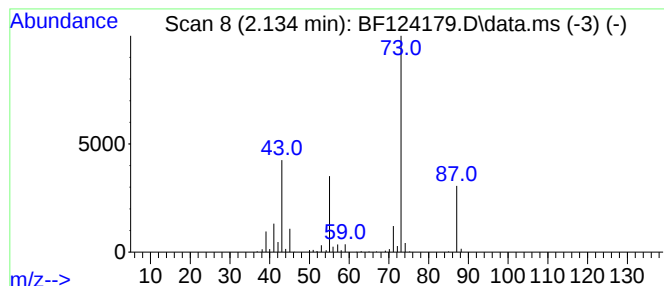
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.134	68.92 ng	791223	1,4-Dichlorobenzene-d4	6.857

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3			2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	25
4			Boronic acid, ethyl-, dimethyl e...	102	C4H11BO2	007318-82-3	12
5			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9



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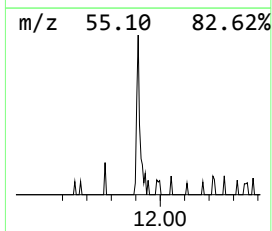
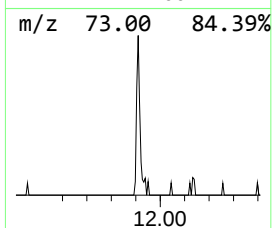
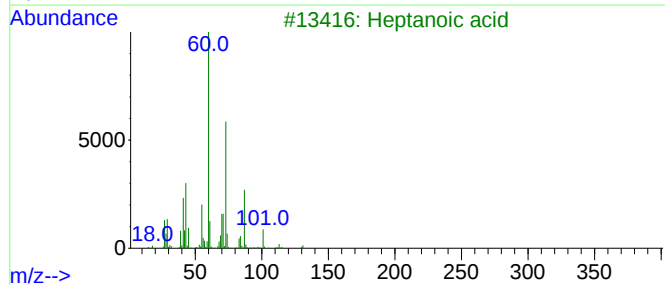
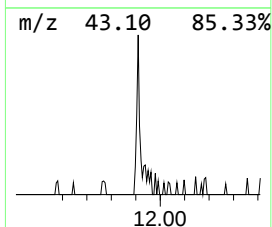
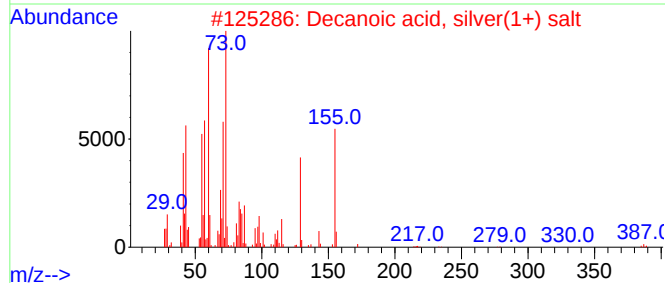
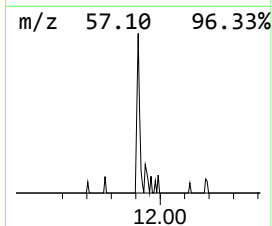
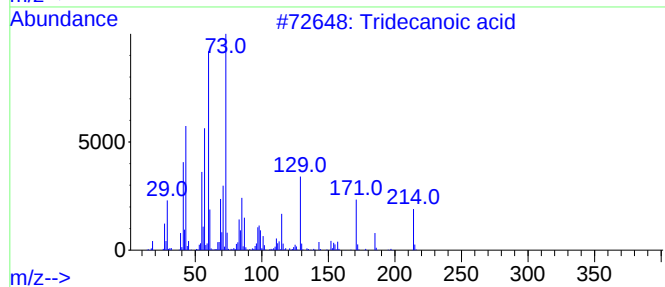
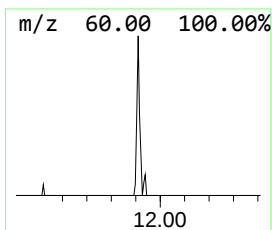
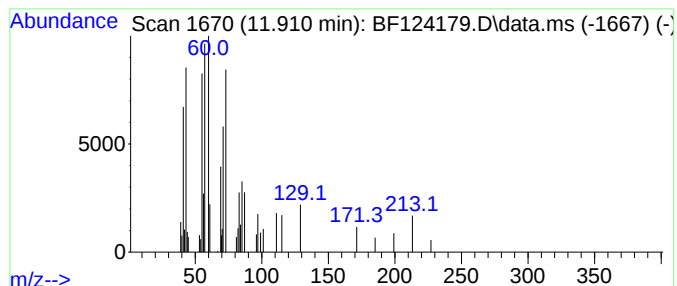
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Peak Number 2 Tridecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.910	2.36 ng	42970	Phenanthrene-d10	11.386

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecanoic acid	214	C13H26O2	000638-53-9	64
2			Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	59
3			Heptanoic acid	130	C7H14O2	000111-14-8	43
4			Oxalic acid, cyclobutyl tetradec...	340	C20H36O4	1000309-70-9	11
5			Undecane, 4,7-dimethyl-	184	C13H28	017301-32-5	10



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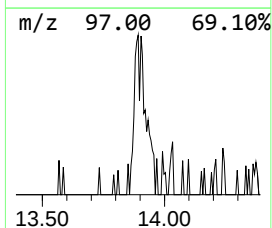
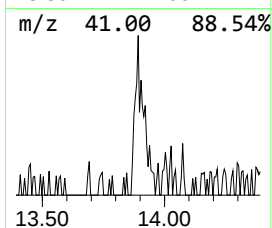
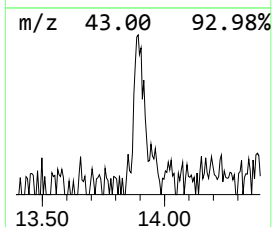
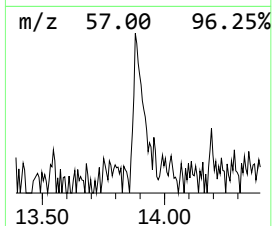
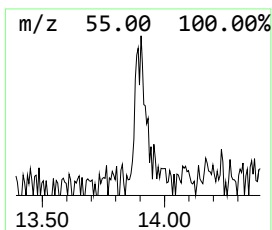
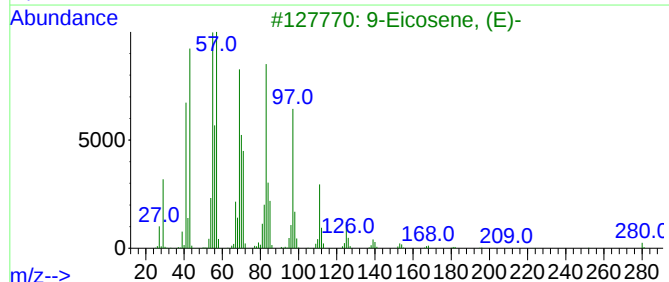
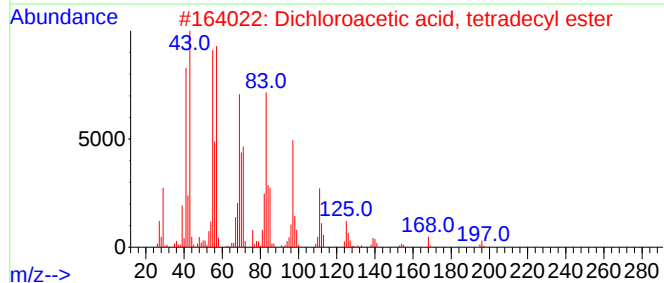
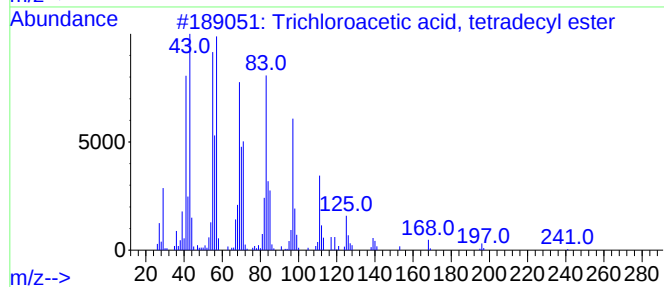
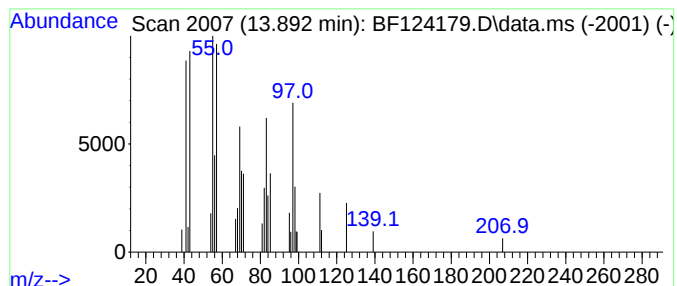
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Peak Number 3 Trichloroacetic acid, tetra... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.892	6.63 ng	112840	Chrysene-d12	14.027

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	83
2			Dichloroacetic acid, tetradecyl ...	324	C16H30Cl2O2	083005-02-1	83
3			9-Eicosene, (E)-	280	C20H40	074685-29-3	81
4			1-Nonadecene	266	C19H38	018435-45-5	80
5			5-Eicosene, (E)-	280	C20H40	074685-30-6	80



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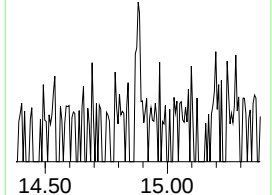
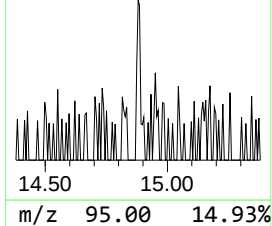
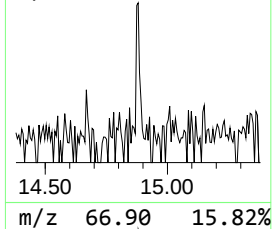
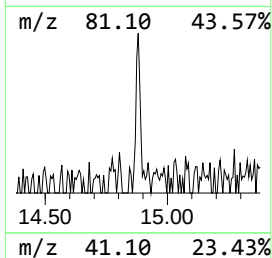
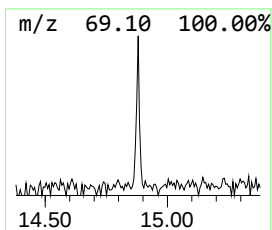
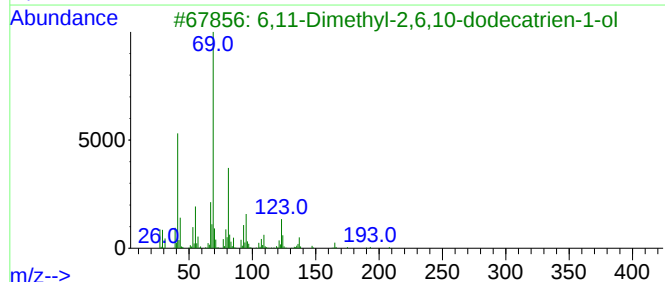
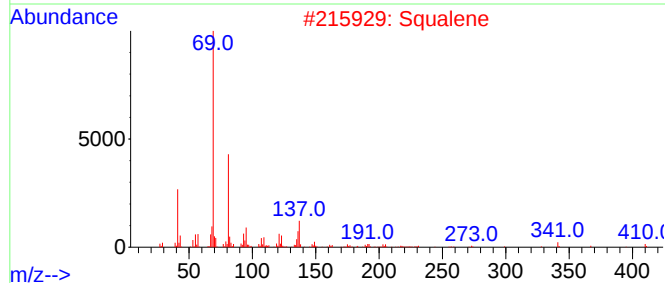
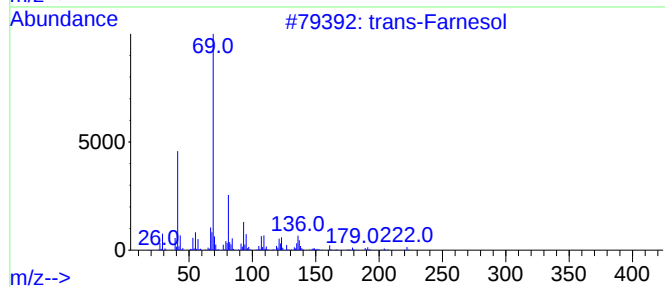
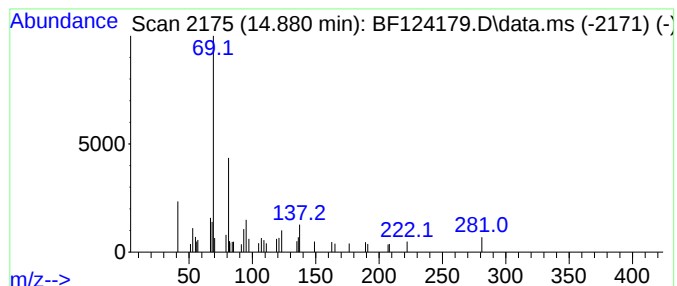
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Peak Number 4 trans-Farnesol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.880	2.43 ng	32398	Perylene-d12	15.509

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			trans-Farnesol	222	C15H26O	000106-28-5	76
2			Squalene	410	C30H50	000111-02-4	72
3			6,11-Dimethyl-2,6,10-dodecatrien...	208	C14H24O	1000196-53-3	64
4			Supraene	410	C30H50	007683-64-9	64
5			2,6,10-Dodecatrienal, 3,7,11-tri...	220	C15H24O	000502-67-0	59



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.134	68.9	ng	791223	1	6.857	229612	20.0
Tridecanoic acid	11.910	2.4	ng	42970	4	11.386	364594	20.0
Trichloroacetic...	13.892	6.6	ng	112840	5	14.027	340374	20.0
trans-Farnesol	14.880	2.4	ng	32398	6	15.509	266641	20.0