

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP060921\
 Data File : BP005813.D
 Acq On : 09 Jun 2021 17:26
 Operator : CG/JU
 Sample : M2650-03
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 DELAWANNA-RT10-STOCKPILE-3

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_P\Methods\8270E-BP060821.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP005813.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.128	4	7	19	rVB	35532	57847	1.54%	0.317%
2	5.052	328	334	343	rVB	111881	165670	4.41%	0.908%
3	5.517	407	413	424	rBV	961808	1373587	36.53%	7.529%
4	7.116	677	685	699	rBV	858364	1386944	36.88%	7.602%
5	7.952	821	827	836	rBV	264320	426501	11.34%	2.338%
6	9.116	1016	1025	1033	rBV	537730	878651	23.37%	4.816%
7	10.757	1295	1304	1313	rBV	322078	552913	14.70%	3.031%
8	13.210	1714	1721	1734	rBV	1355180	2010260	53.46%	11.019%
9	14.034	1850	1861	1871	rBV	220831	327557	8.71%	1.795%
10	14.581	1947	1954	1962	rVB	494007	727961	19.36%	3.990%
11	16.063	2199	2206	2221	rBV	1239532	1862213	49.52%	10.208%
12	17.322	2413	2420	2427	rBV	667572	917325	24.39%	5.028%
13	18.204	2564	2570	2579	rBV	258064	382343	10.17%	2.096%
14	19.063	2710	2716	2725	rBV5	14411	40609	1.08%	0.223%
15	19.428	2775	2778	2784	rBV2	52619	76046	2.02%	0.417%
16	19.869	2847	2853	2862	rBV	3130845	3760508	100.00%	20.613%
17	20.151	2897	2901	2910	rBV5	26459	45850	1.22%	0.251%
18	21.104	3058	3063	3070	rBV	332587	486420	12.93%	2.666%
19	21.392	3107	3112	3117	rBV	989207	1274409	33.89%	6.986%
20	23.816	3518	3524	3532	rVB2	719234	1489736	39.62%	8.166%

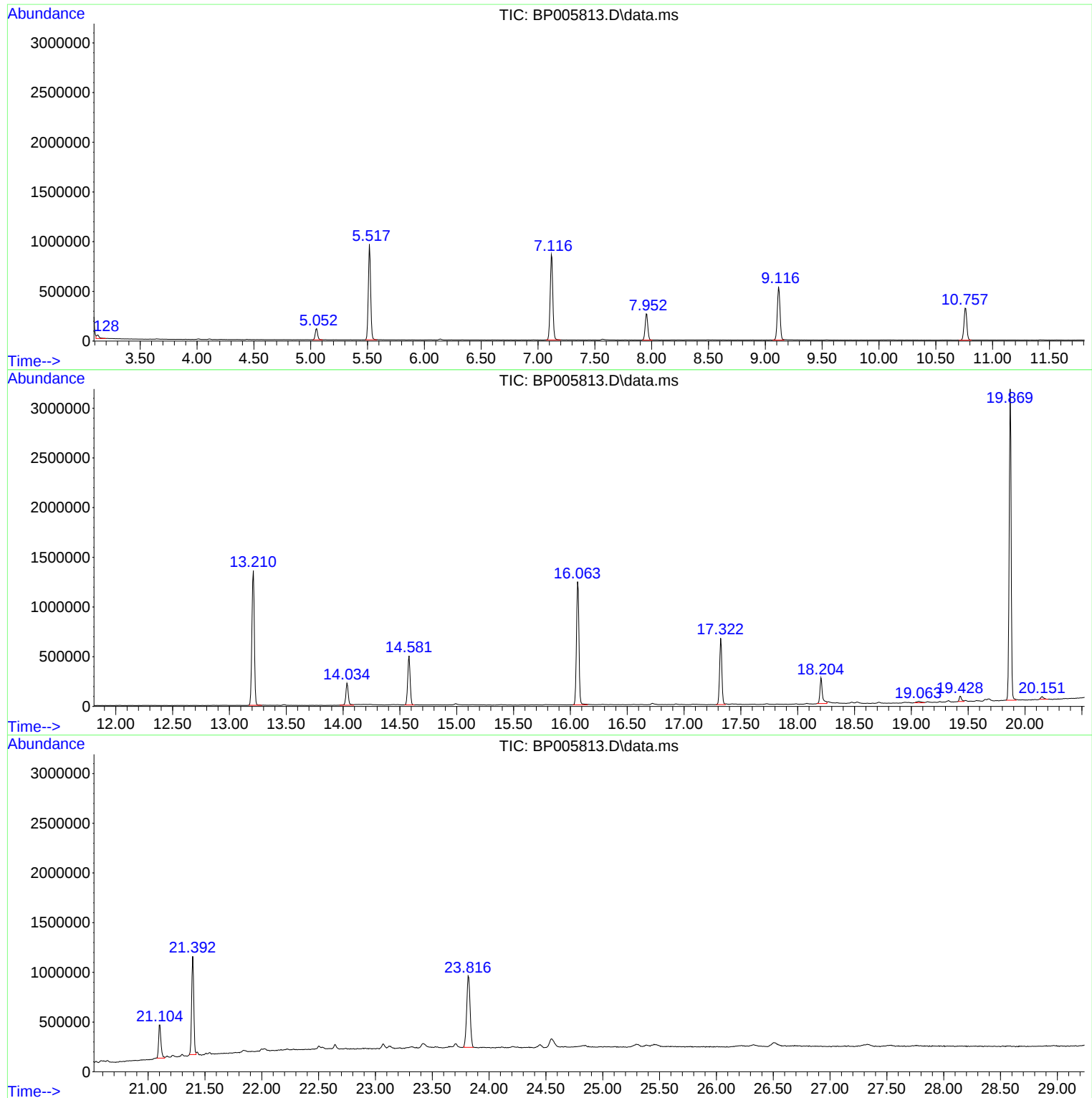
Sum of corrected areas: 18243350

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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP060821.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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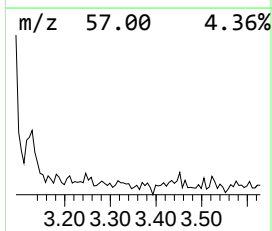
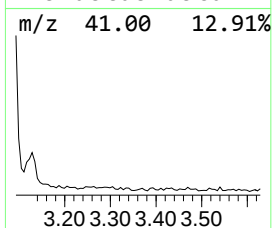
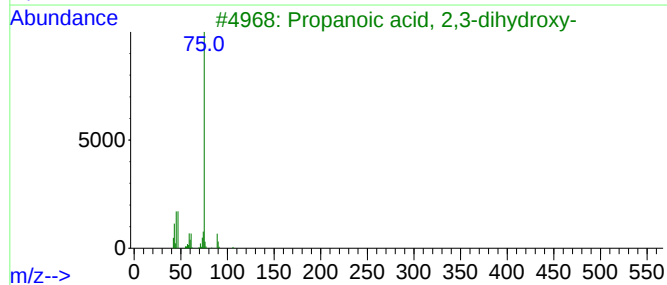
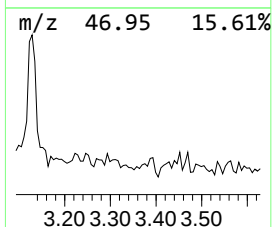
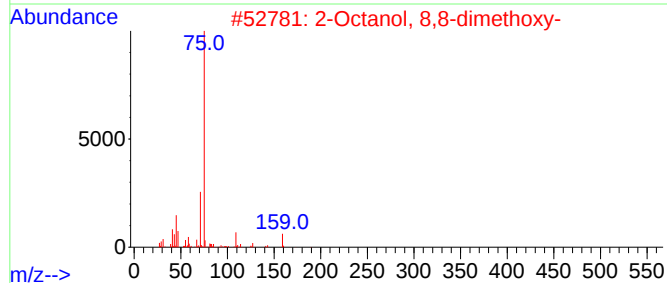
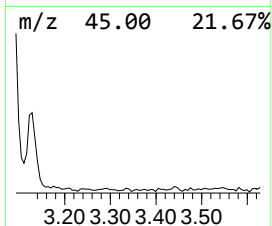
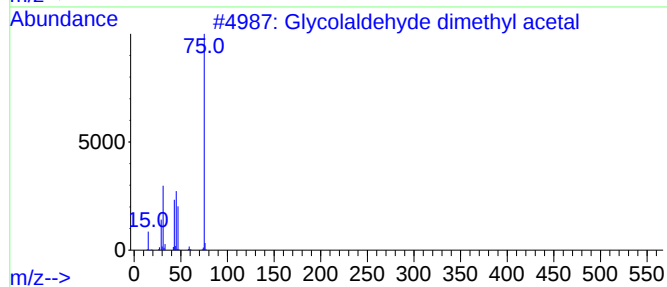
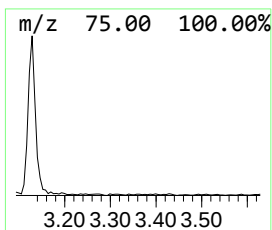
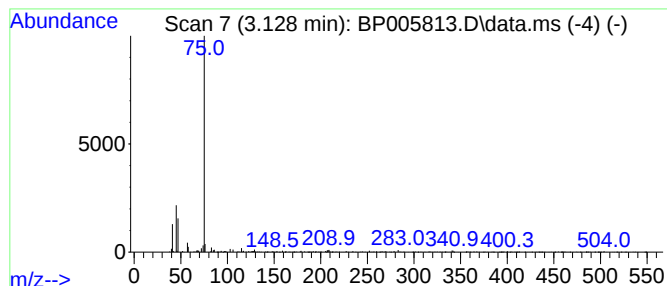
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP060821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown3.128 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.128	2.71 ng	57847	1,4-Dichlorobenzene-d4	7.952

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Glycolaldehyde dimethyl acetal	106	C4H10O3	030934-97-5	40
2			2-Octanol, 8,8-dimethoxy-	190	C10H22O3	312305-55-8	40
3			Propanoic acid, 2,3-dihydroxy-	106	C3H6O4	000473-81-4	9
4			3-(Methylthio)-2-butanone	118	C5H10O3	053475-15-3	9
5			3-Bromopropionaldehyde dimethyl ...	182	C5H11BrO2	036255-44-4	9



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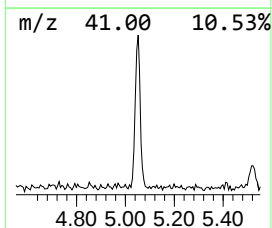
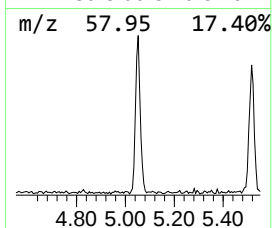
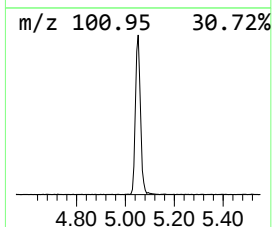
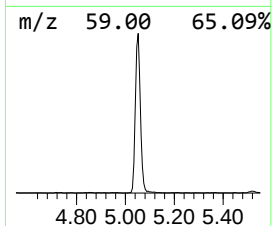
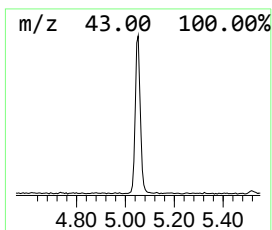
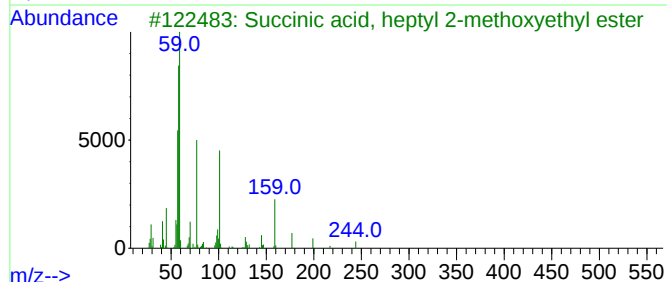
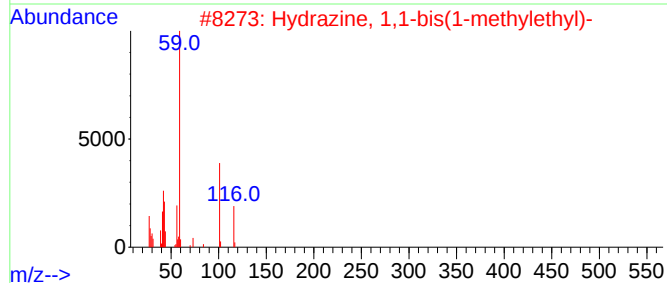
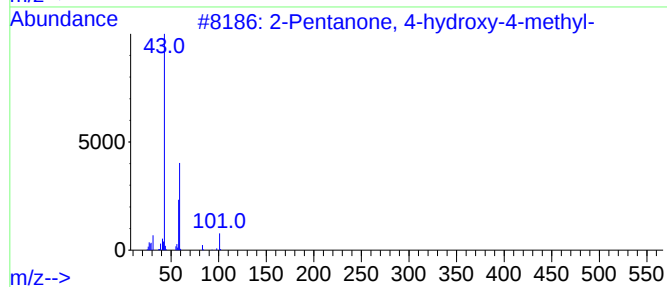
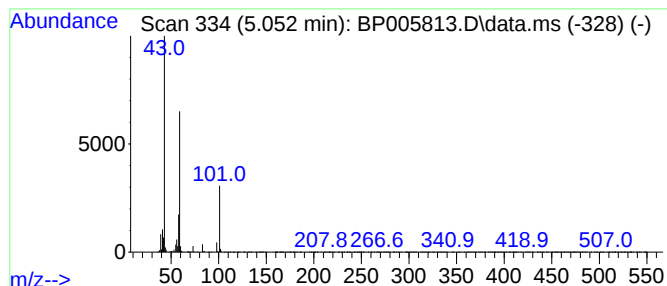
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.052	7.77 ng	165670	1,4-Dichlorobenzene-d4	7.952

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2			Hydrazine, 1,1-bis(1-methylethyl)-	116	C6H16N2	000921-14-2	38
3			Succinic acid, heptyl 2-methoxye...	274	C14H26O5	1000325-80-7	28
4			3-Tridecanol	200	C13H28O	010289-68-6	25
5			(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	25



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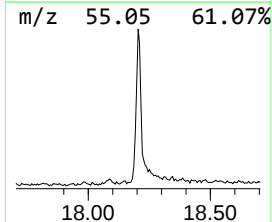
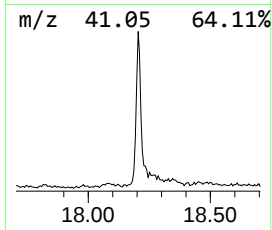
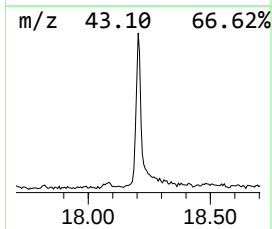
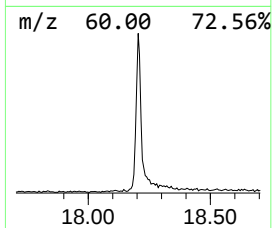
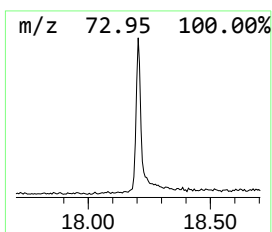
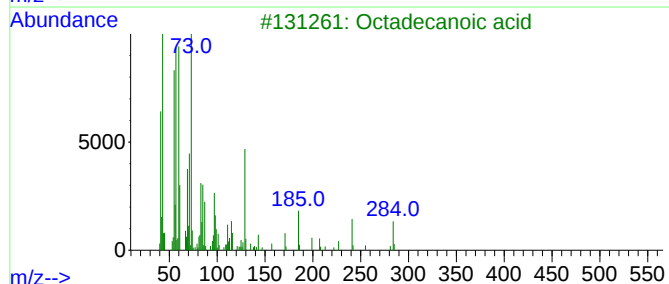
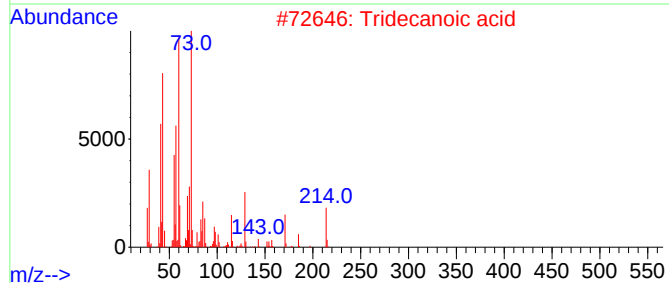
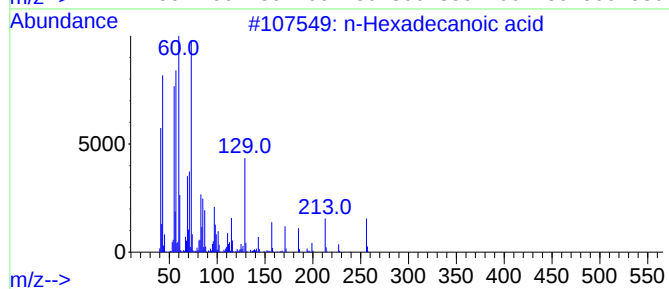
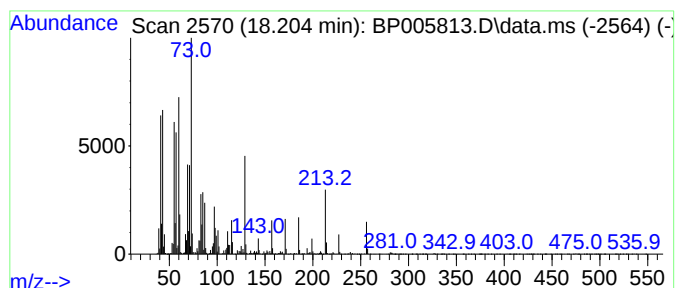
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.204	8.34 ng	382343	Phenanthrene-d10	17.322

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tridecanoic acid	214	C13H26O2	000638-53-9	86
3			Octadecanoic acid	284	C18H36O2	000057-11-4	81
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	74
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	64



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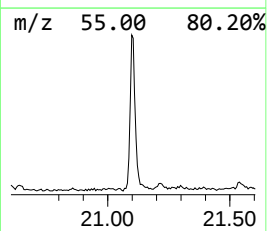
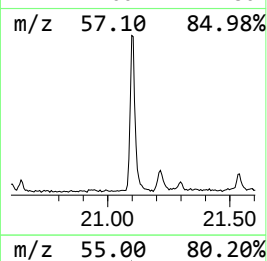
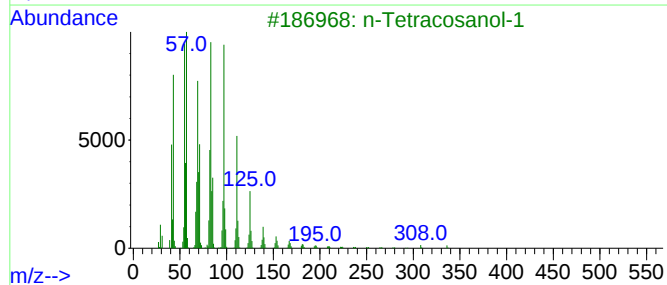
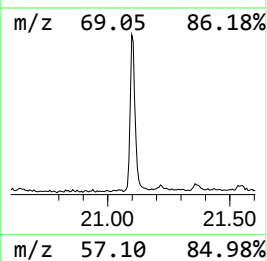
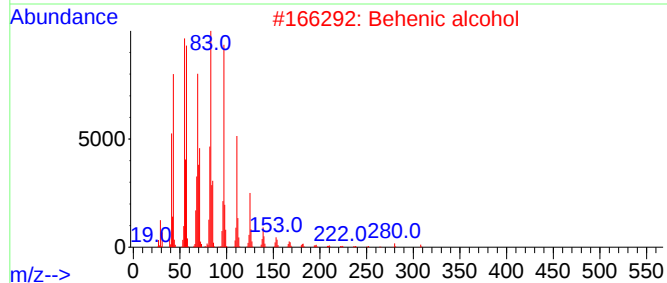
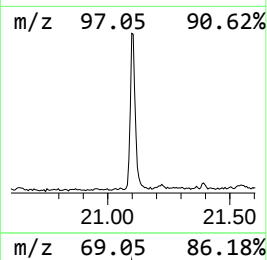
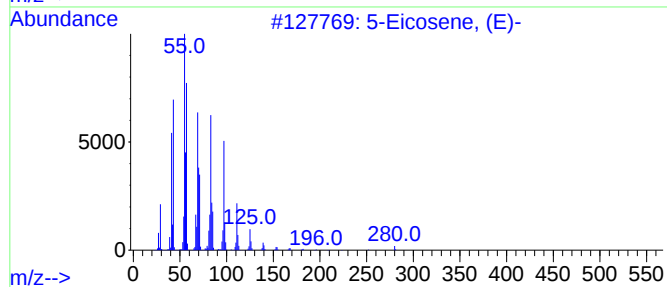
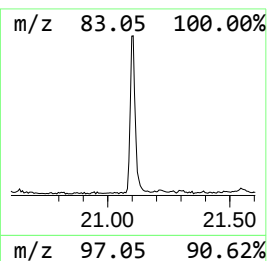
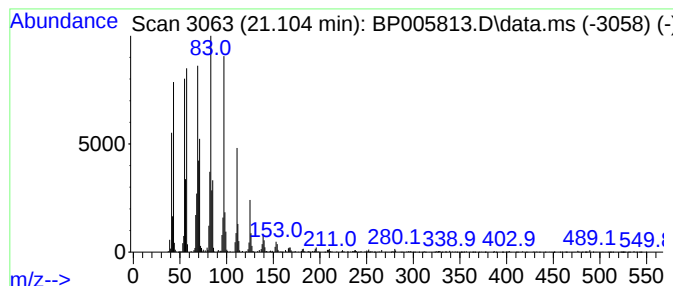
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Peak Number 4 5-Eicosene, (E)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.104	7.63 ng	486420	Chrysene-d12	21.392

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			5-Eicosene, (E)-	280	C20H40	074685-30-6	98
2			Behenic alcohol	326	C22H46O	000661-19-8	95
3			n-Tetracosanol-1	354	C24H50O	000506-51-4	93
4			Nonadecyl trifluoroacetate	380	C21H39F3O2	1000351-76-3	93
5			n-Nonadecanol-1	284	C19H40O	001454-84-8	93



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown3.128	3.128	2.7	ng	57847	1	7.952	426501	20.0
2-Pentanone, 4-...	5.052	7.8	ng	165670	1	7.952	426501	20.0
n-Hexadecanoic ...	18.204	8.3	ng	382343	4	17.322	917325	20.0
5-Eicosene, (E)-	21.104	7.6	ng	486420	5	21.392	1274410	20.0