

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF032421\
 Data File : BF123444.D
 Acq On : 24 Mar 2021 17:50
 Operator : JU/CG
 Sample : M1770-02
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MW-106I

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-BF032321.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF123444.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.246	20	27	32	rVB	3494770	4540136	59.81%	10.356%
2	2.352	40	45	51	rBV	158983	194201	2.56%	0.443%
3	5.134	511	518	525	rVB	122507	150708	1.99%	0.344%
4	5.528	581	585	588	rBV	3667739	3425164	45.13%	7.813%
5	6.528	750	755	760	rBV	2499166	2319923	30.56%	5.292%
6	6.910	817	820	824	rBV	1592706	1364393	17.98%	3.112%
7	7.475	910	916	919	rBV	4398119	4558854	60.06%	10.399%
8	8.198	1034	1039	1042	rBV	2069375	1767645	23.29%	4.032%
9	9.281	1217	1223	1226	rBV	7306605	7590352	100.00%	17.314%
10	9.663	1285	1288	1292	rBV	110707	108411	1.43%	0.247%
11	9.957	1334	1338	1341	rBV	2364213	1923730	25.34%	4.388%
12	10.751	1467	1473	1476	rBV	5147706	4897681	64.53%	11.172%
13	11.445	1587	1591	1595	rBV	2057291	1785229	23.52%	4.072%
14	11.975	1677	1681	1684	rBV2	173013	156870	2.07%	0.358%
15	12.433	1752	1759	1762	rBV	118566	99634	1.31%	0.227%
16	13.045	1858	1863	1866	rBV	6266245	6206027	81.76%	14.156%
17	13.939	2011	2015	2023	rBV	561354	551497	7.27%	1.258%
18	14.092	2037	2041	2045	rBV	1072984	1051609	13.85%	2.399%
19	15.604	2292	2298	2302	rBV	892192	1147006	15.11%	2.616%

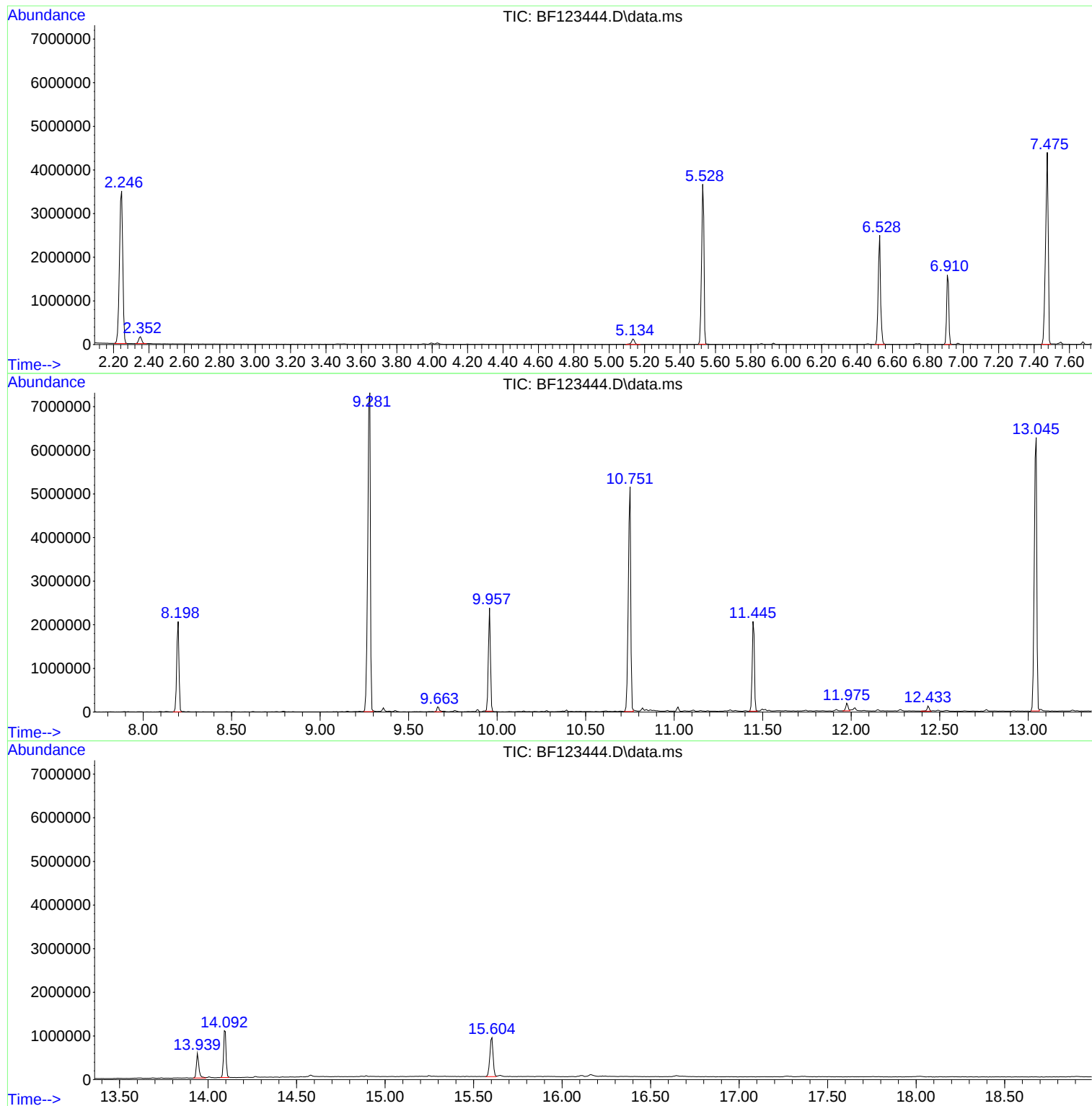
Sum of corrected areas: 43839070

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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF032321.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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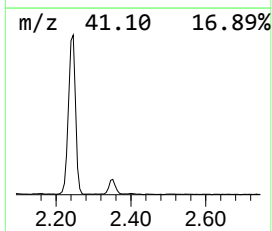
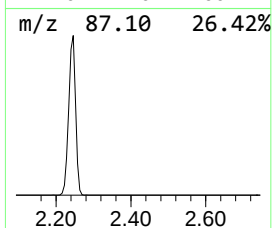
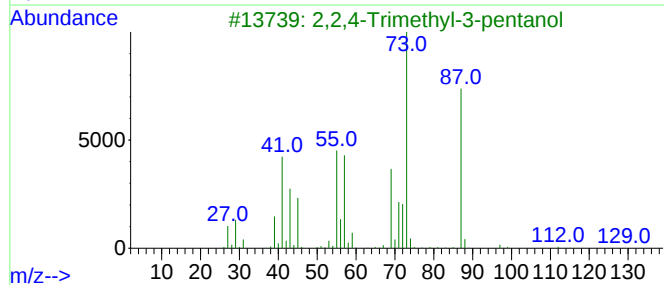
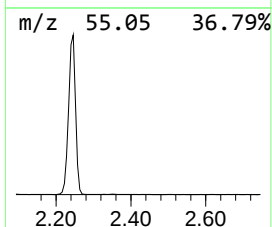
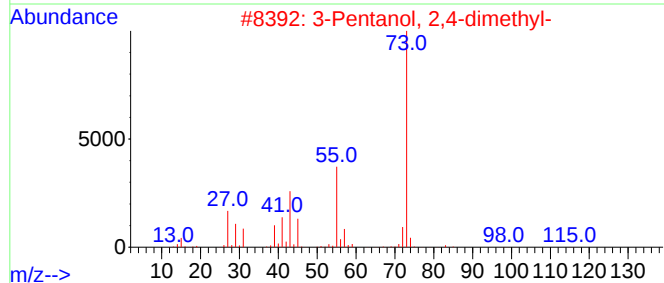
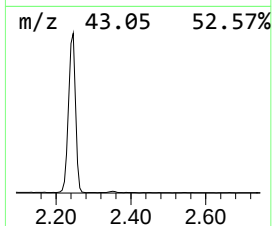
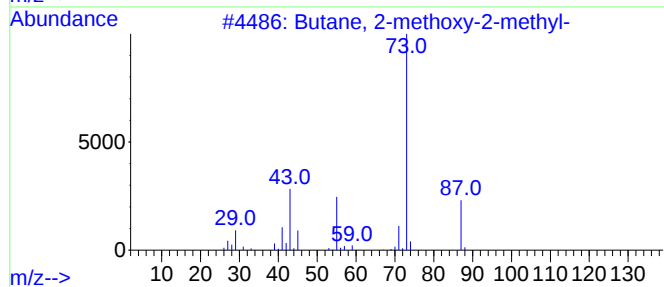
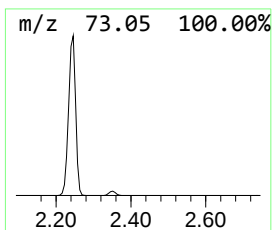
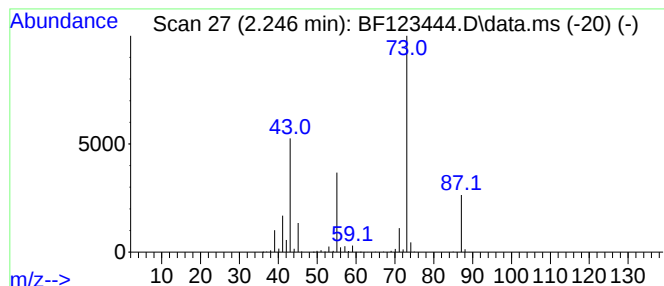
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF032321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.246	66.55 ng	4540140	1,4-Dichlorobenzene-d4	6.910

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	43
3			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
4			Silane, tetramethyl-	88	C4H12Si	000075-76-3	38
5			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23



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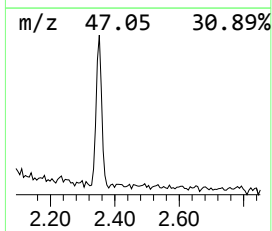
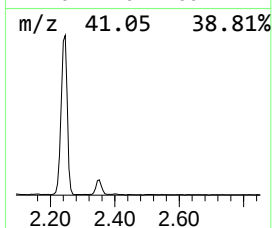
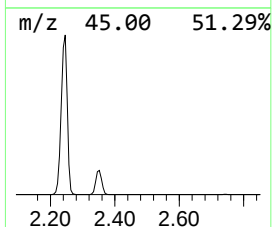
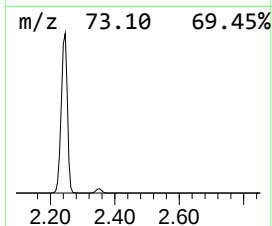
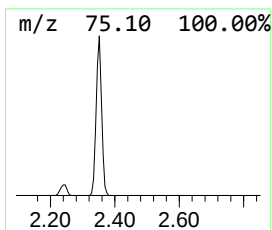
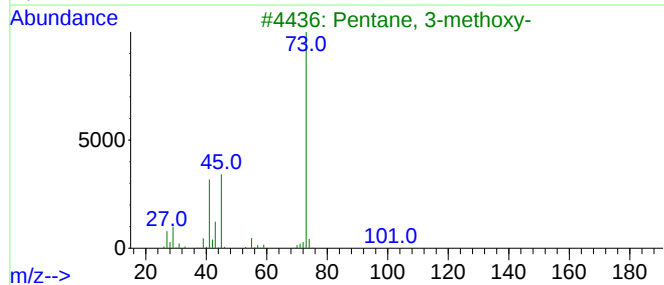
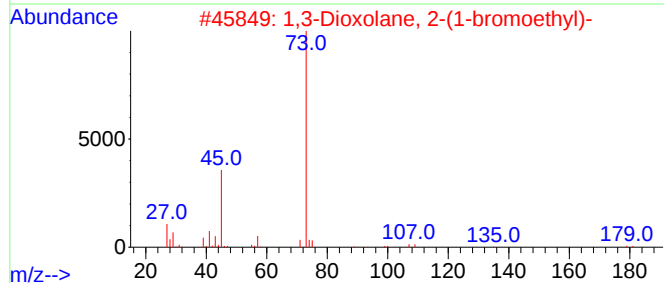
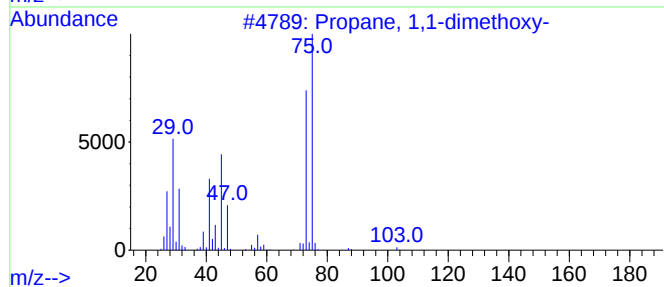
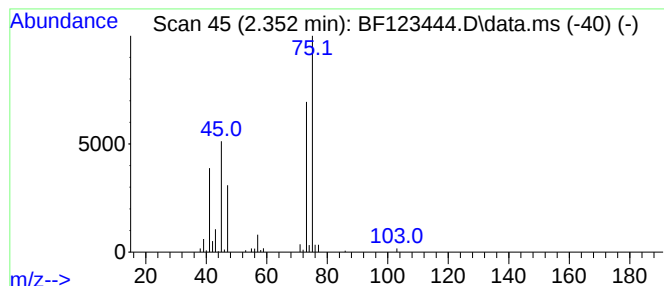
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TIC Integration Parameters: LSCINT.P

Peak Number 2 Propane, 1,1-dimethoxy- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.352	2.85 ng	194201	1,4-Dichlorobenzene-d4	6.910

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	72
2			1,3-Dioxolane, 2-(1-bromoethyl)-	180	C5H9BrO2	005267-73-2	22
3			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	22
4			1-Cyclohexyl-3-ethoxy-butan-2-one	198	C12H22O2	074897-69-1	10
5			Ethanamine, 2-propoxy-	103	C5H13NO	042185-03-5	9



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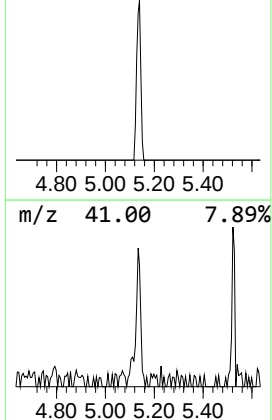
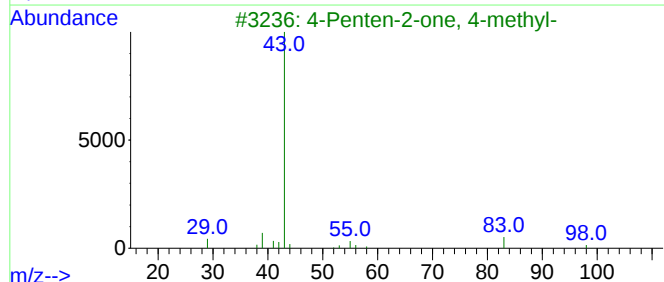
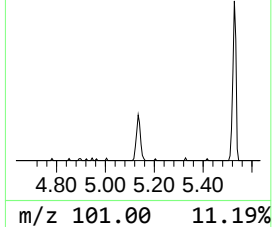
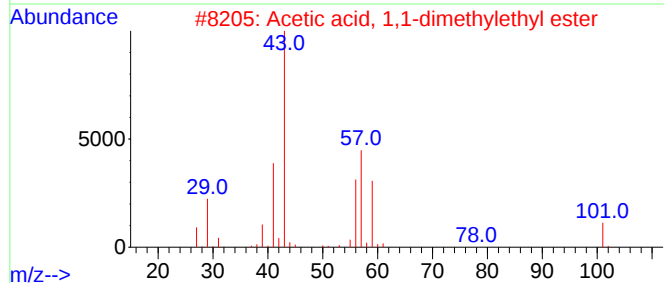
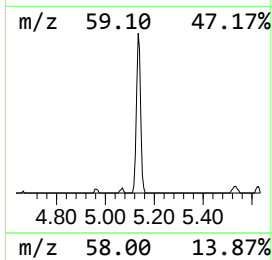
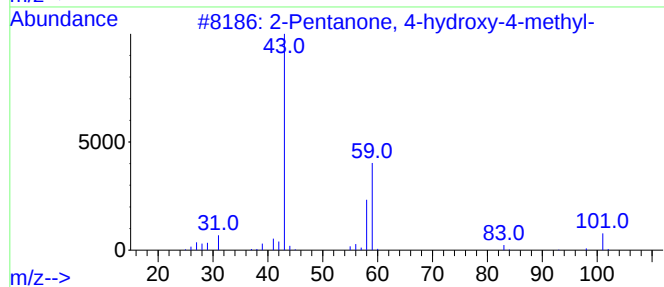
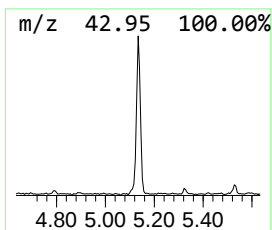
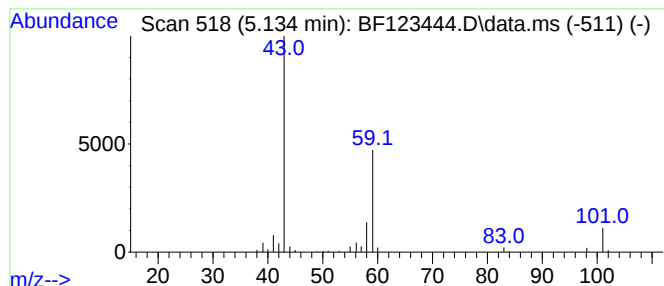
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Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.134	2.21 ng	150708	1,4-Dichlorobenzene-d4	6.910

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50		
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	28		
3	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	9		
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9		
5	2-Pentanone, 5-(acetyloxy)-	144	C7H12O3	005185-97-7	9		



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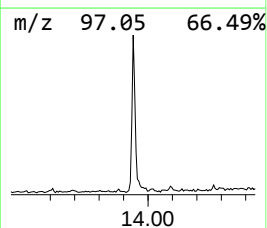
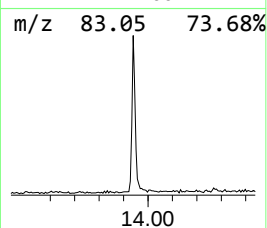
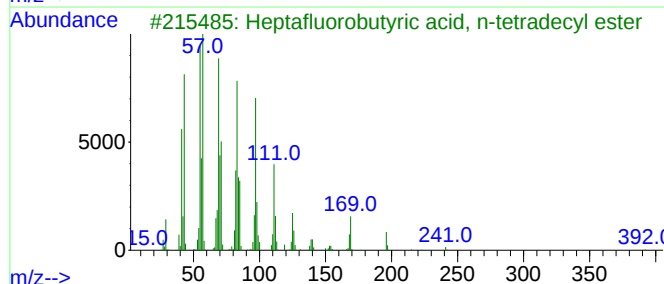
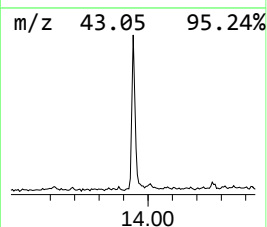
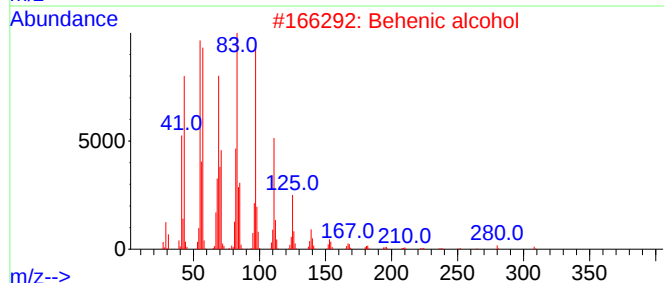
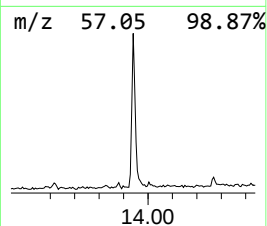
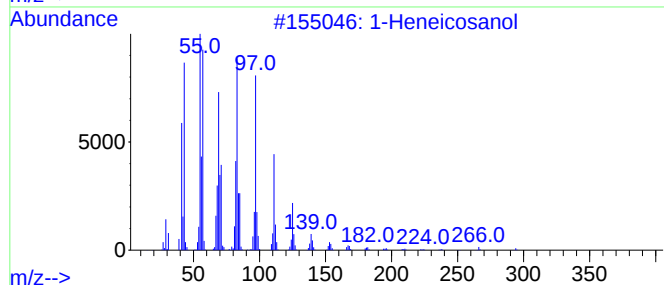
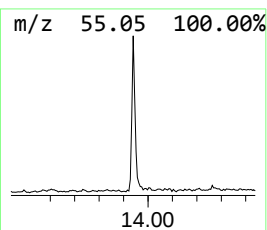
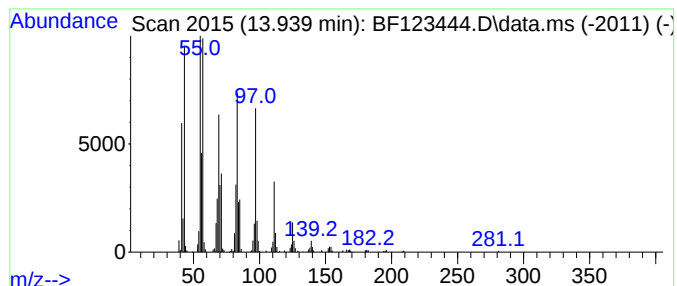
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Peak Number 4 1-Heneicosanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.939	10.49 ng	551497	Chrysene-d12	14.098

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Heneicosanol	312	C21H44O	015594-90-8	94
2			Behenic alcohol	326	C22H46O	000661-19-8	93
3			Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	91
4			1-Octadecanol	270	C18H38O	000112-92-5	91
5			Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	91



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.246	66.5	ng	4540140	1	6.910	1364390	20.0
Propane, 1,1-di...	2.352	2.9	ng	194201	1	6.910	1364390	20.0
2-Pentanone, 4-...	5.134	2.2	ng	150708	1	6.910	1364390	20.0
1-Heneicosanol	13.939	10.5	ng	551497	5	14.098	1051610	20.0