

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP062421\
 Data File : BP006058.D
 Acq On : 24 Jun 2021 18:03
 Operator : CG/JU
 Sample : M2812-07
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 KG-WATER

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: BP006058.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.016	323	328	339	rBV	53194	79363	2.12%	0.501%
2	5.487	401	408	420	rBV	614699	932574	24.97%	5.886%
3	7.093	674	681	699	rBV	377362	666218	17.84%	4.205%
4	7.910	813	820	828	rBV	259977	418634	11.21%	2.642%
5	9.075	1011	1018	1029	rBV	573005	1011707	27.08%	6.386%
6	10.510	1255	1262	1276	rBV2	19375	52755	1.41%	0.333%
7	10.716	1289	1297	1311	rBV	304688	541469	14.50%	3.418%
8	13.169	1706	1714	1730	rBV	1620762	2387936	63.93%	15.073%
9	14.539	1940	1947	1956	rBV	469778	692958	18.55%	4.374%
10	16.028	2194	2200	2221	rBV	1124758	1694539	45.36%	10.696%
11	17.286	2408	2414	2424	rBV	562210	816343	21.85%	5.153%
12	18.169	2559	2564	2573	rBV	108231	167062	4.47%	1.054%
13	19.398	2769	2773	2780	rBV3	40960	65323	1.75%	0.412%
14	19.833	2842	2847	2856	rBV	3204140	3735424	100.00%	23.578%
15	21.057	3052	3055	3064	rBV2	158590	229179	6.14%	1.447%
16	21.133	3065	3068	3075	rVV	99551	130913	3.50%	0.826%
17	21.363	3102	3107	3112	rBV	771355	1029533	27.56%	6.498%
18	23.763	3509	3515	3527	rVB2	574631	1190926	31.88%	7.517%

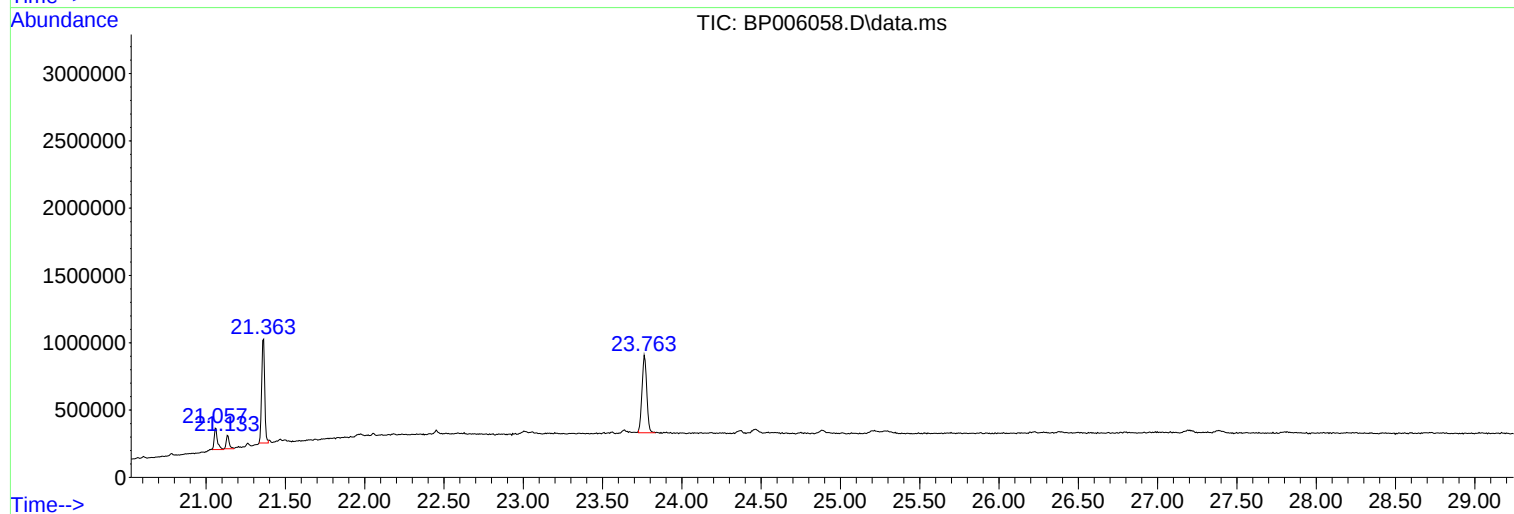
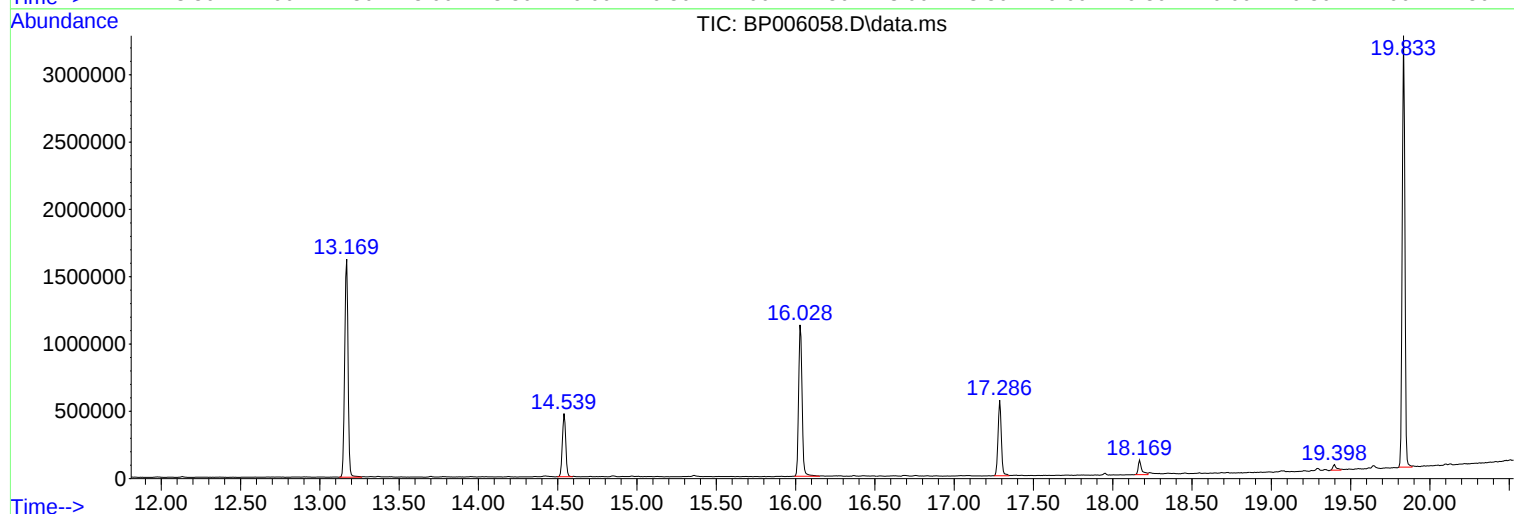
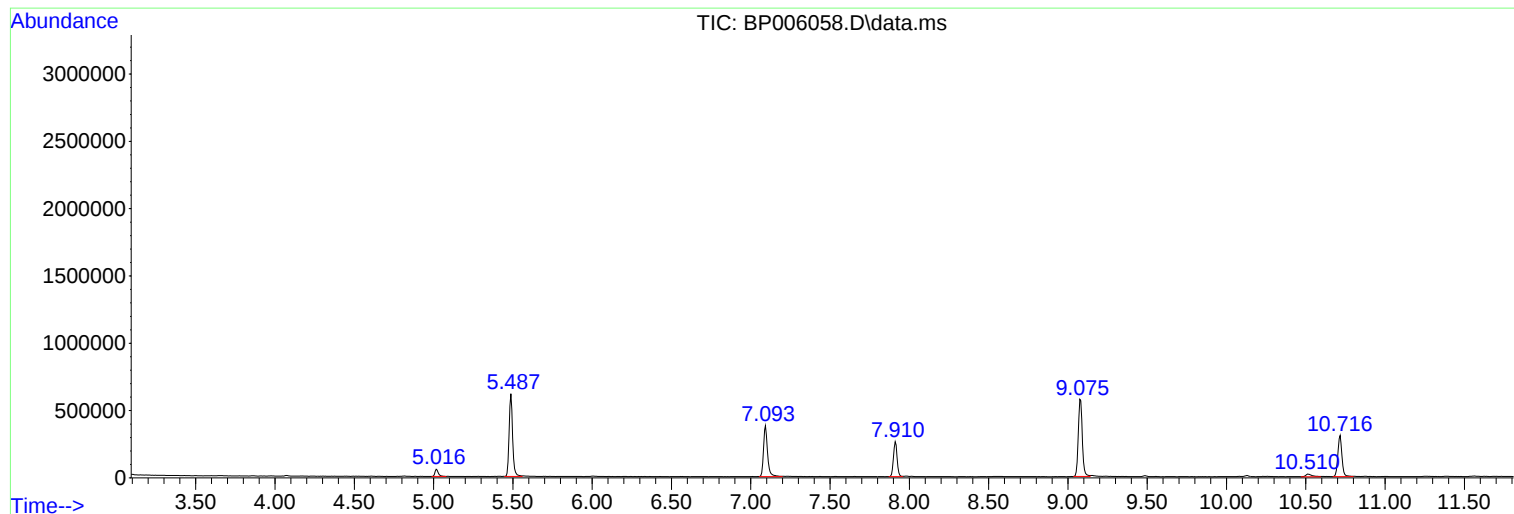
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP060821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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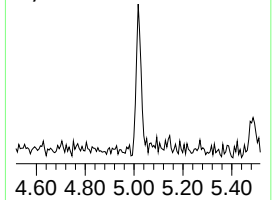
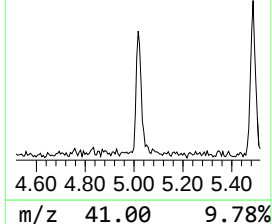
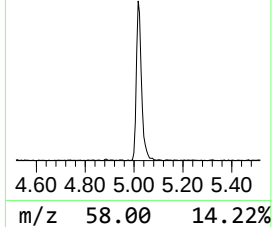
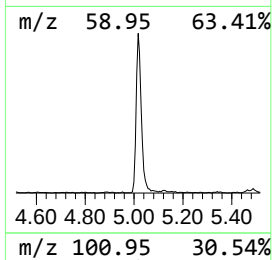
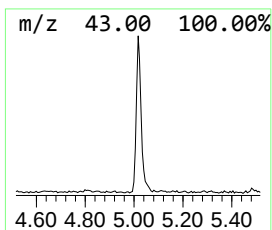
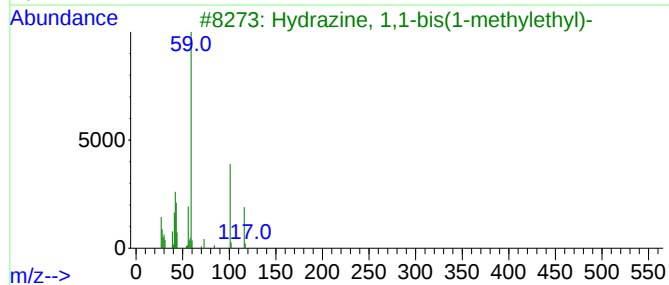
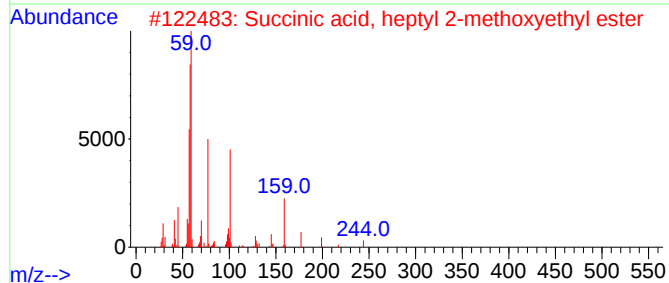
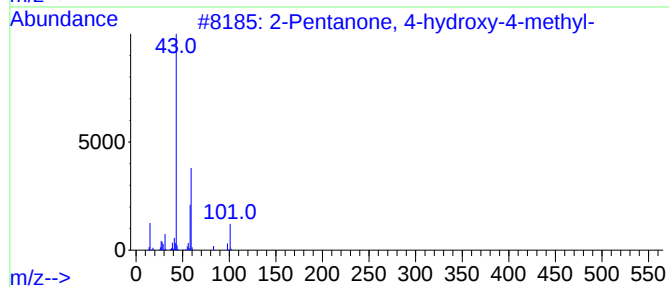
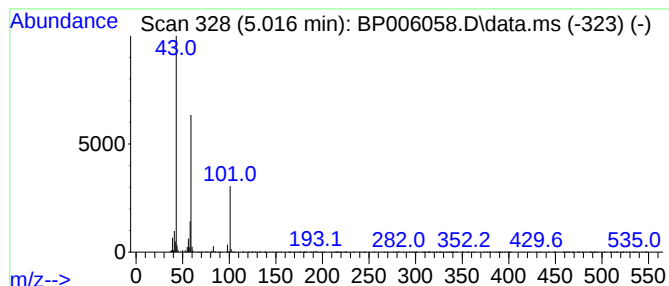
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.016	3.79 ng	79363	1,4-Dichlorobenzene-d4	7.910

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			Succinic acid, heptyl 2-methoxye...	274	C14H26O5	1000325-80-7	33
3			Hydrazine, 1,1-bis(1-methylethyl)-	116	C6H16N2	000921-14-2	28
4			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
5			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	17



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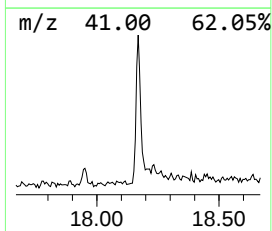
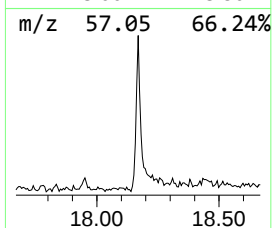
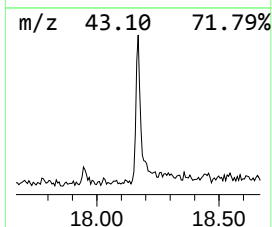
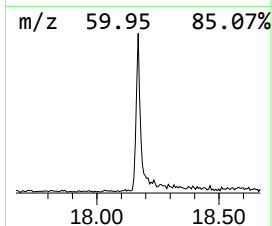
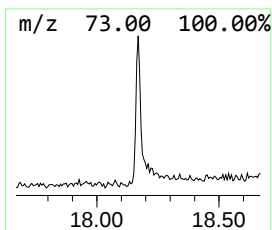
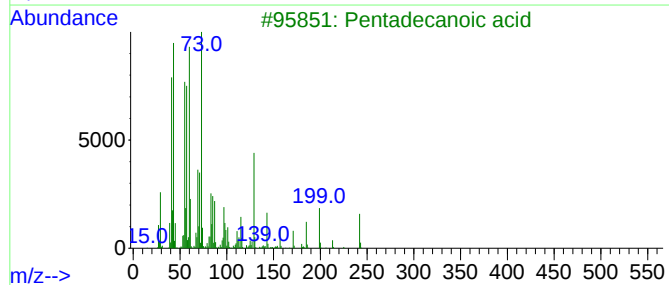
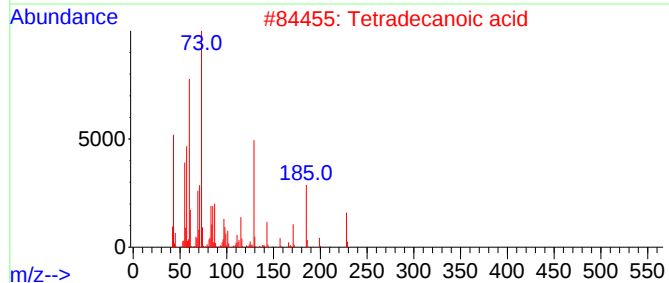
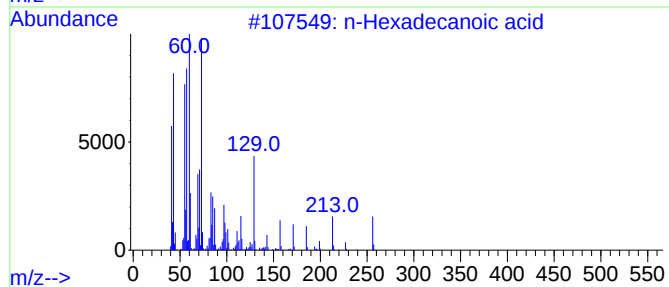
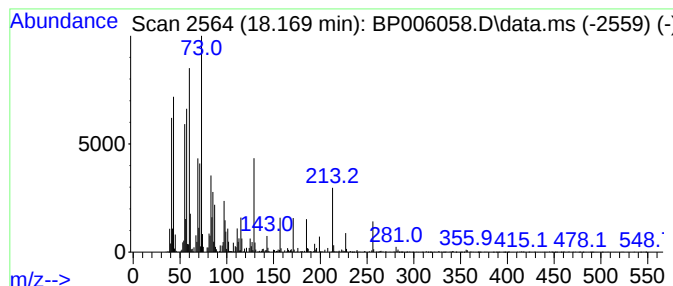
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 2 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.169	4.09 ng	167062	Phenanthrene-d10	17.286

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2		Tetradecanoic acid	228	C14H28O2	000544-63-8	86
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	83
4		n-Decanoic acid	172	C10H20O2	000334-48-5	76
5		Undecanoic acid	186	C11H22O2	000112-37-8	72



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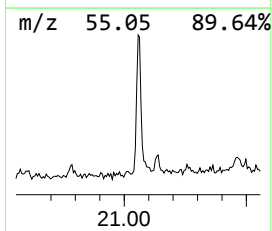
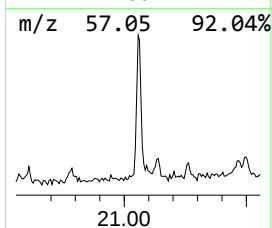
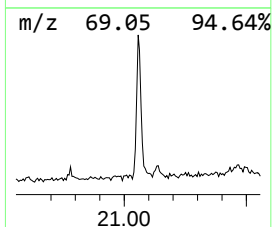
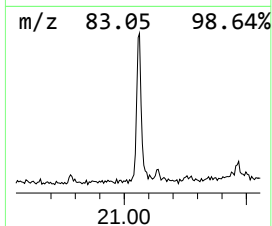
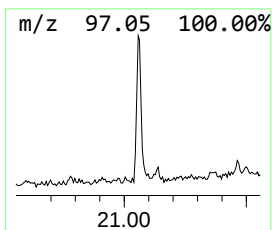
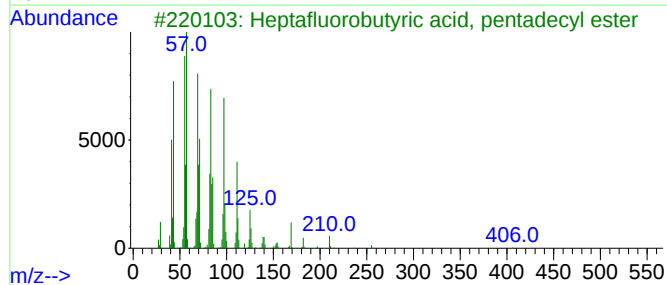
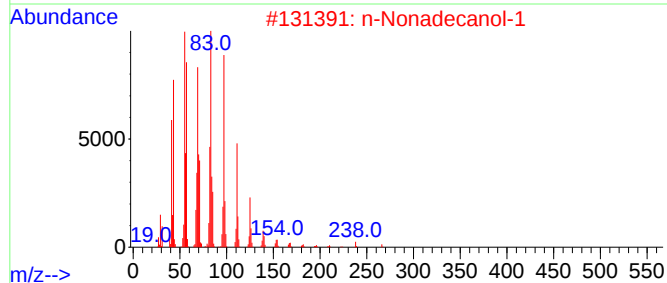
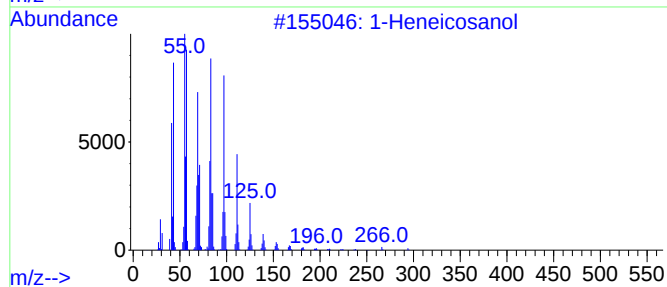
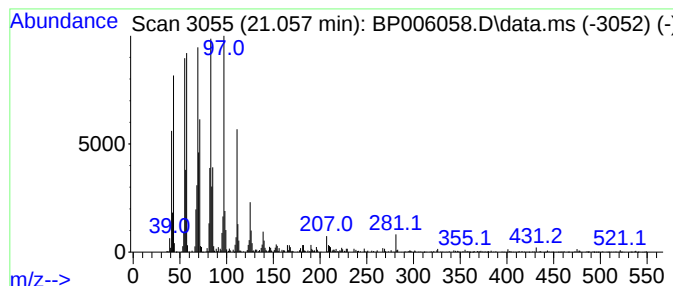
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Peak Number 3 1-Heneicosanol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.057	4.45 ng	229179	Chrysene-d12	21.363

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Heneicosanol	312	C21H44O	015594-90-8	93
2			n-Nonadecanol-1	284	C19H40O	001454-84-8	93
3			Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	91
4			3-Eicosene, (E)-	280	C20H40	074685-33-9	91
5			Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	91



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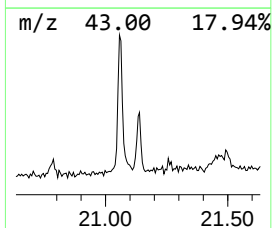
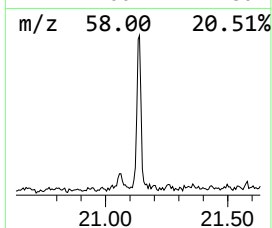
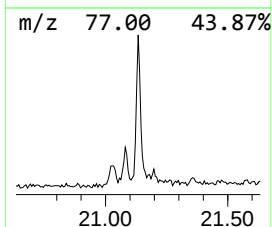
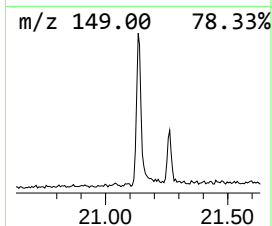
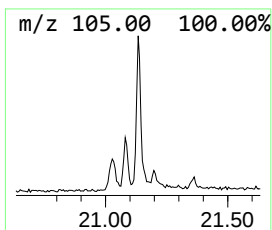
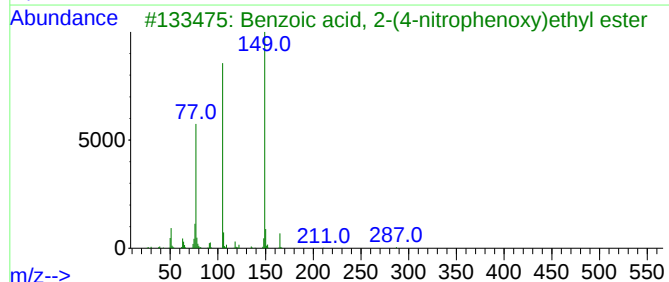
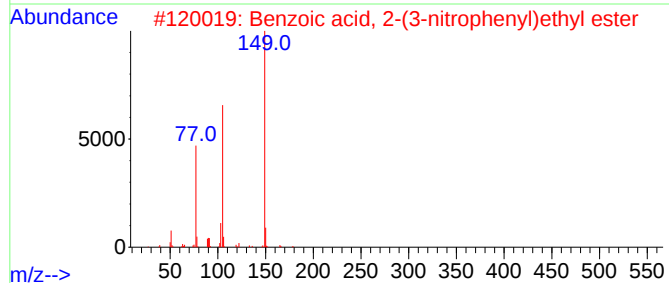
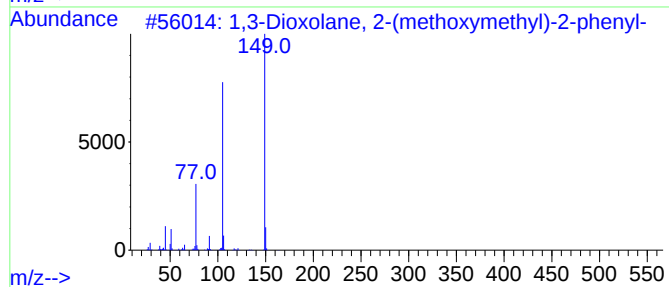
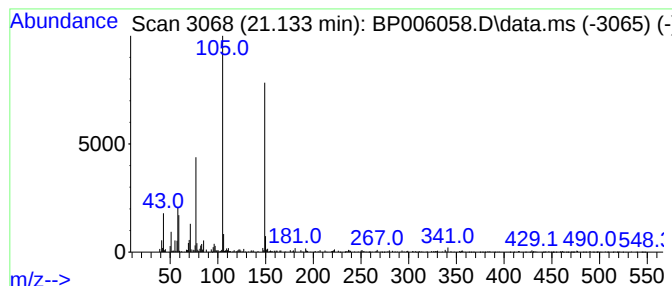
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Peak Number 4 1,3-Dioxolane, 2-(methoxyme... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.133	2.54 ng	130913	Chrysene-d12	21.363

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Dioxolane, 2-(methoxymethyl)...	194	C11H14O3	1000156-71-2	59		
2	Benzoic acid, 2-(3-nitrophenyl)e...	271	C15H13NO4	1000368-22-4	59		
3	Benzoic acid, 2-(4-nitrophenoxy)...	287	C15H13NO5	1000368-92-7	53		
4	Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	52		
5	Phthalic acid, dodecyl 2-methoxy...	392	C23H36O5	1000315-80-8	50		



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.016	3.8	ng	79363	1	7.910	418634	20.0
n-Hexadecanoic ...	18.169	4.1	ng	167062	4	17.286	816343	20.0
1-Heneicosanol	21.057	4.5	ng	229179	5	21.363	1029530	20.0
1,3-Dioxolane, ...	21.133	2.5	ng	130913	5	21.363	1029530	20.0