

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP030722\
 Data File : BP009291.D
 Acq On : 07 Mar 2022 18:26
 Operator : CG/JU
 Sample : N1806-09
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 DUM-26

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-BP030522.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP009291.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.075	11	15	31	rVB	1097534	1699923	7.20%	1.273%
2	5.416	406	413	431	rBV	8559809	13741656	58.22%	10.289%
3	6.993	672	681	700	rBV	8225856	13922930	58.99%	10.425%
4	7.822	814	822	830	rBV	1811809	3082365	13.06%	2.308%
5	8.975	1009	1018	1031	rBV	5066087	8933684	37.85%	6.689%
6	10.610	1287	1296	1310	rBV	2264708	4145650	17.57%	3.104%
7	13.081	1709	1716	1729	rVB	11850915	18947613	80.28%	14.187%
8	14.457	1943	1950	1957	rBV	3288250	5008339	21.22%	3.750%
9	15.951	2196	2204	2216	rBV	9178622	14037488	59.48%	10.511%
10	17.216	2412	2419	2424	rBV	3679665	5625257	23.83%	4.212%
11	17.257	2424	2426	2432	rVB	191756	236811	1.00%	0.177%
12	18.122	2569	2573	2582	rBV	484815	657302	2.79%	0.492%
13	19.233	2757	2762	2771	rBV	573048	902025	3.82%	0.675%
14	19.592	2814	2823	2833	rBV2	500490	1312576	5.56%	0.983%
15	19.798	2852	2858	2868	rVB	16962699	23601026	100.00%	17.672%
16	21.051	3067	3071	3076	rBV	912573	1162938	4.93%	0.871%
17	21.321	3111	3117	3122	rBV	4472607	6557873	27.79%	4.910%
18	21.980	3225	3229	3238	rVB2	321022	553724	2.35%	0.415%
19	22.139	3252	3256	3265	rVB	704871	1090595	4.62%	0.817%
20	23.468	3479	3482	3488	rVB2	300918	479983	2.03%	0.359%
21	23.733	3520	3527	3546	rVB	2982233	6479439	27.45%	4.852%
22	24.992	3736	3741	3753	rVB3	549287	1373541	5.82%	1.028%

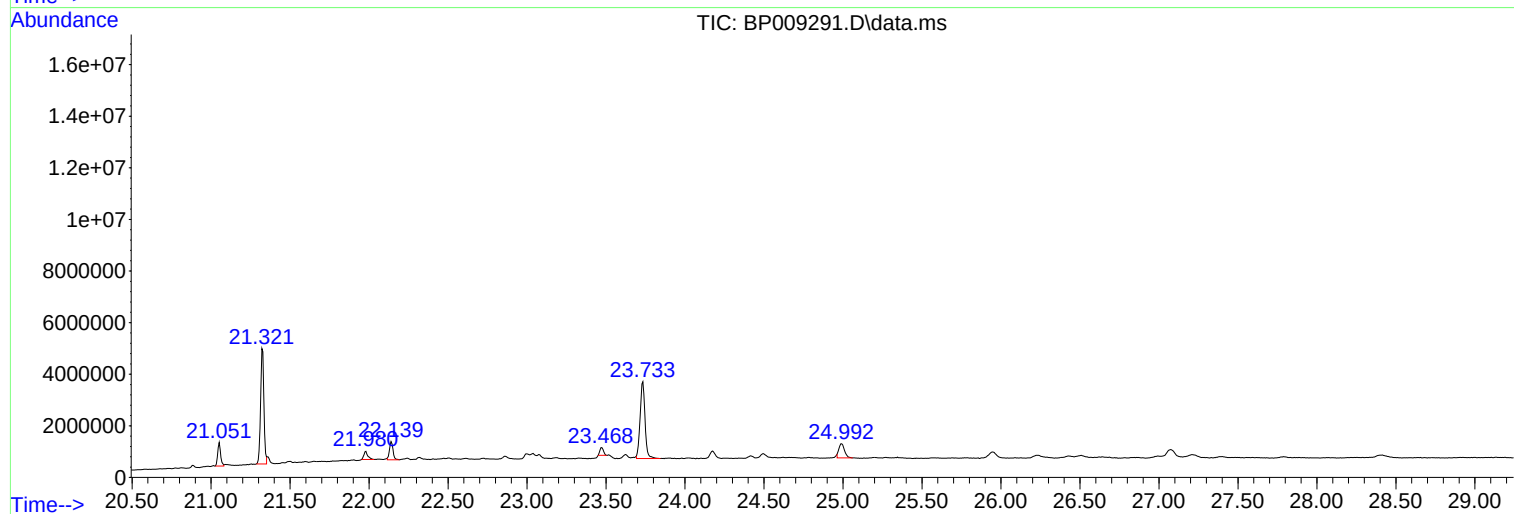
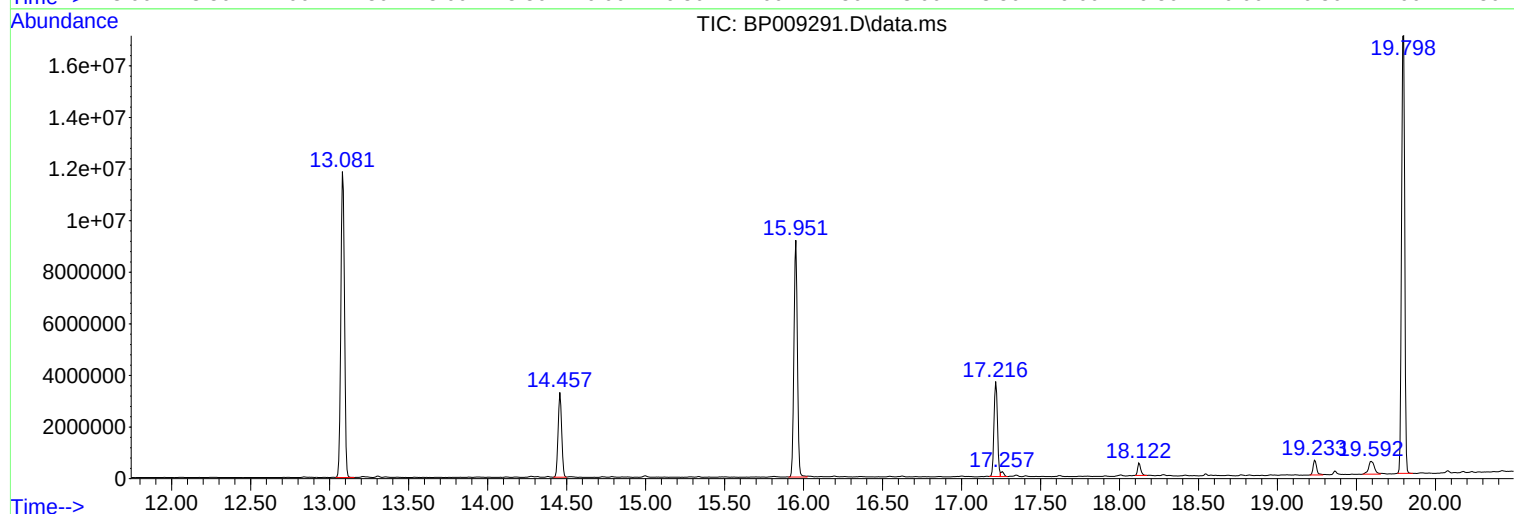
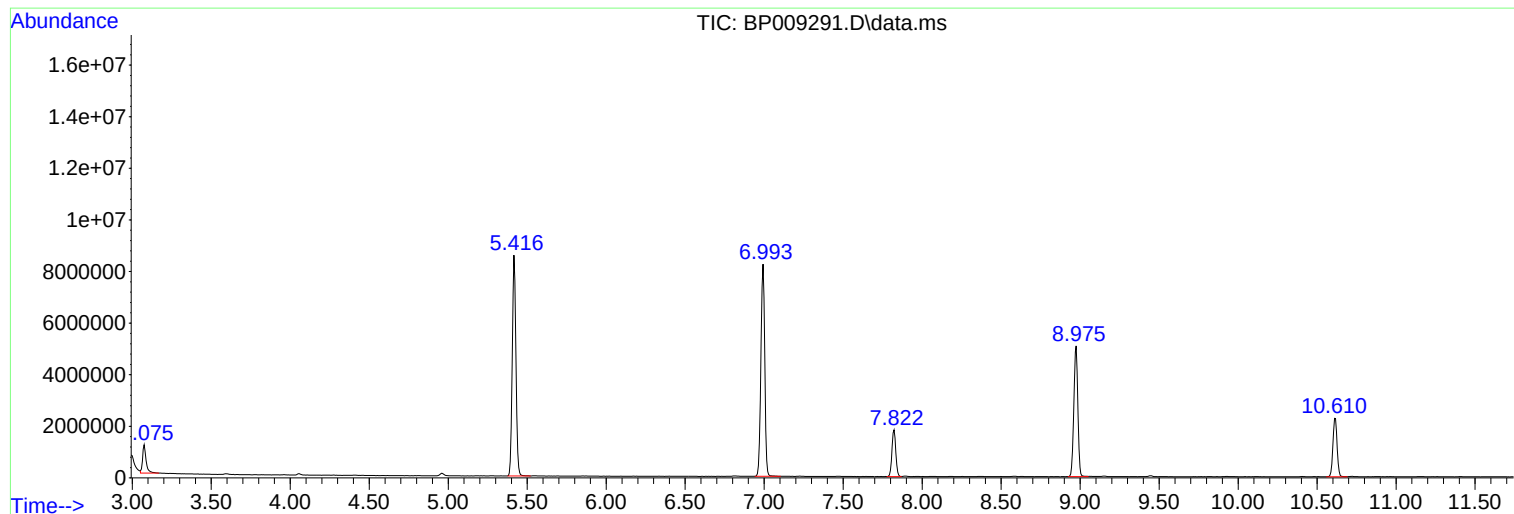
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP030522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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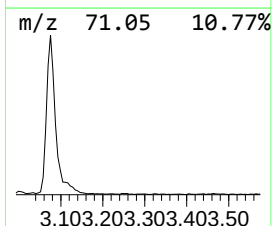
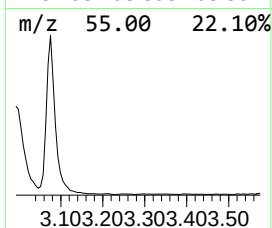
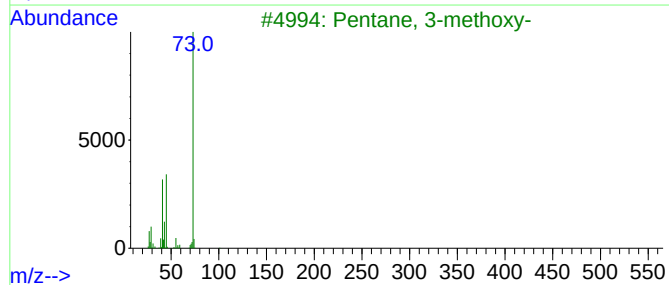
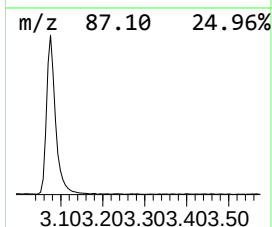
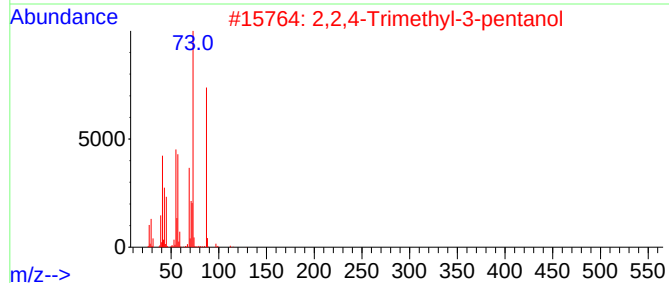
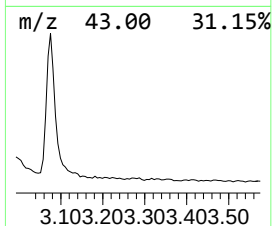
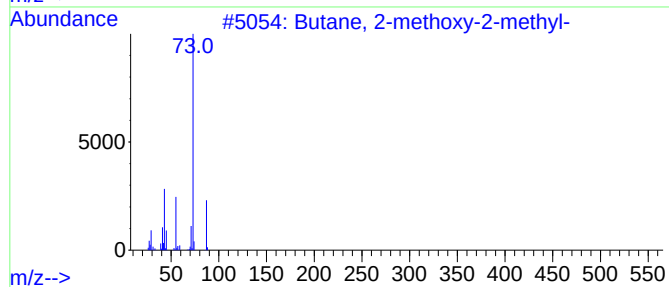
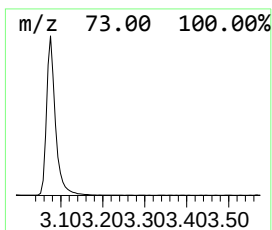
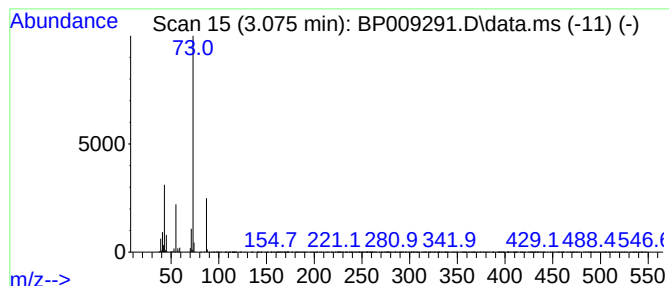
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.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.
3.075	11.03 ng	1699920	1,4-Dichlorobenzene-d4	7.822

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	90
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
4			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	17
5			Silane, tetramethyl-	88	C4H12Si	000075-76-3	9



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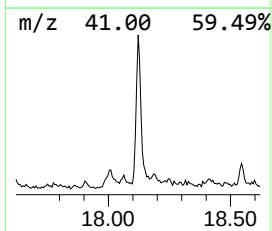
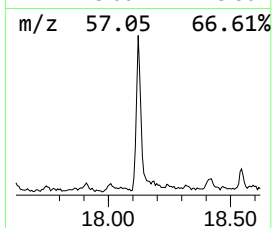
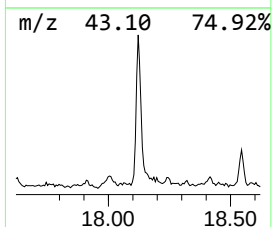
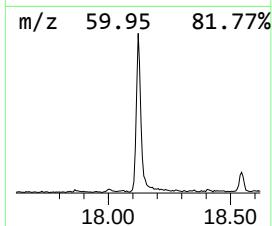
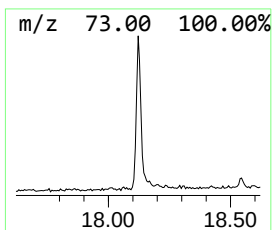
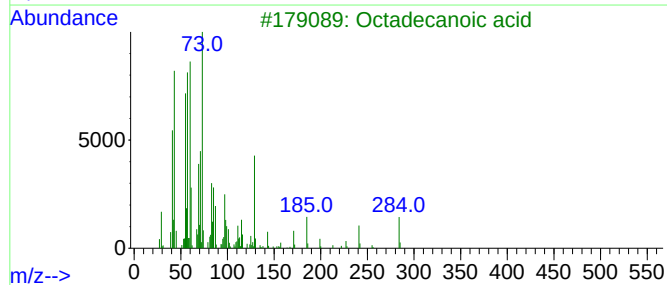
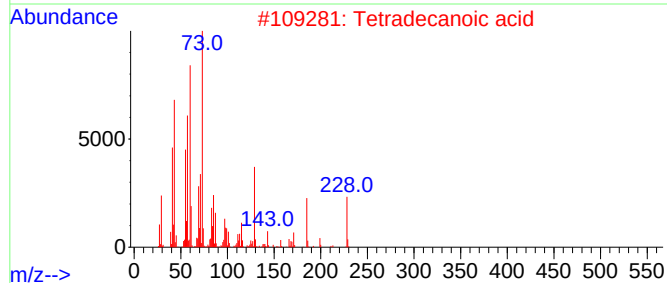
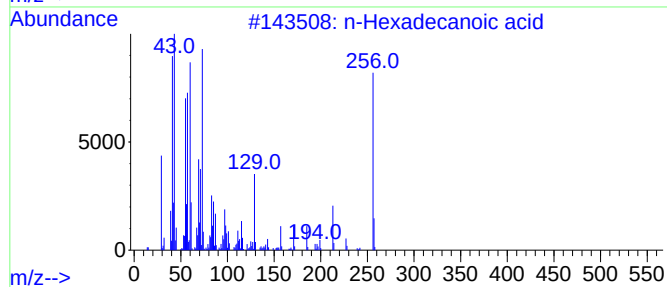
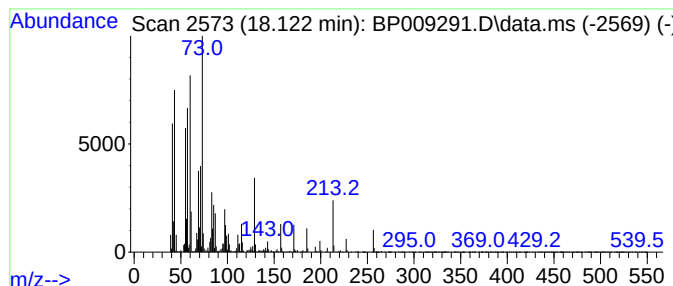
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.122	2.34 ng	657302	Phenanthrene-d10	17.216

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2		Tetradecanoic acid	228	C14H28O2	000544-63-8	86
3		Octadecanoic acid	284	C18H36O2	000057-11-4	81
4		Pentadecanoic acid	242	C15H30O2	001002-84-2	76
5		Tridecanoic acid	214	C13H26O2	000638-53-9	70



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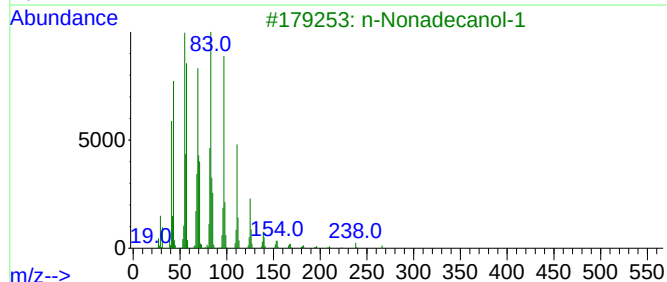
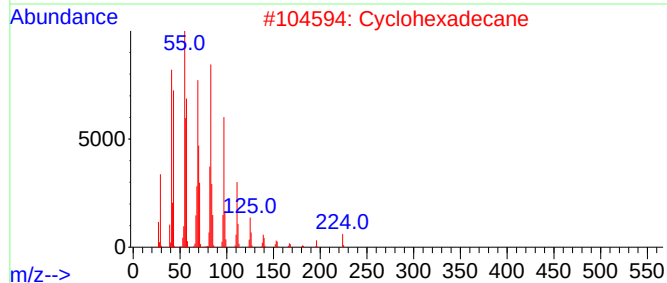
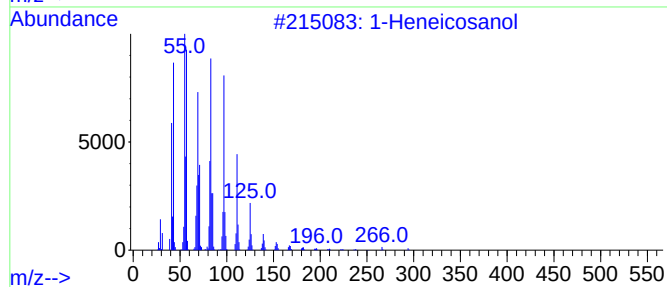
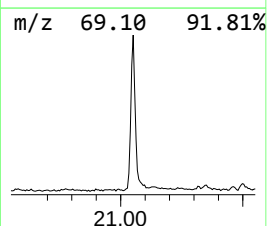
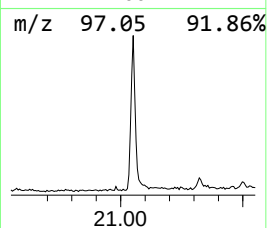
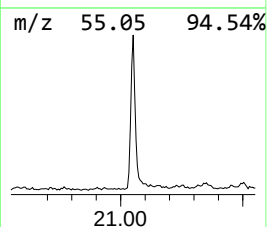
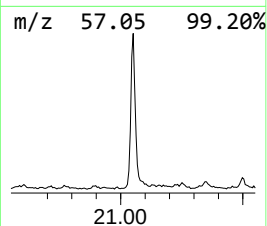
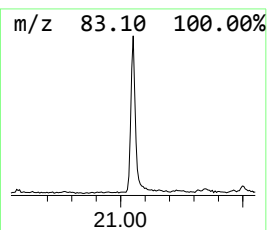
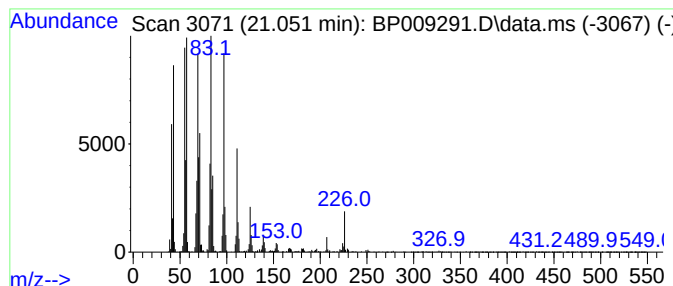
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Peak Number 4 1-Heneicosanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.051	3.55 ng	1162940	Chrysene-d12	21.321

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Heneicosanol	312	C21H44O	015594-90-8	95
2			Cyclohexadecane	224	C16H32	000295-65-8	94
3			n-Nonadecanol-1	284	C19H40O	001454-84-8	94
4			Behenic alcohol	326	C22H46O	000661-19-8	94
5			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94



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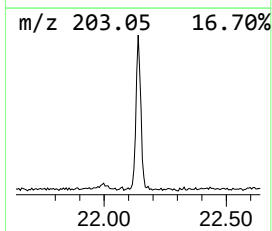
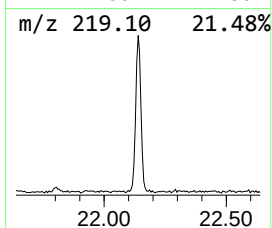
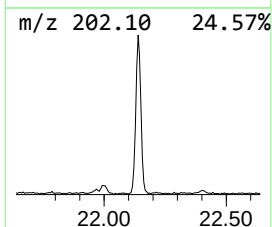
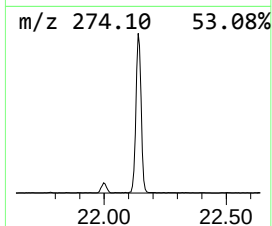
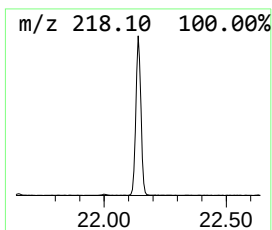
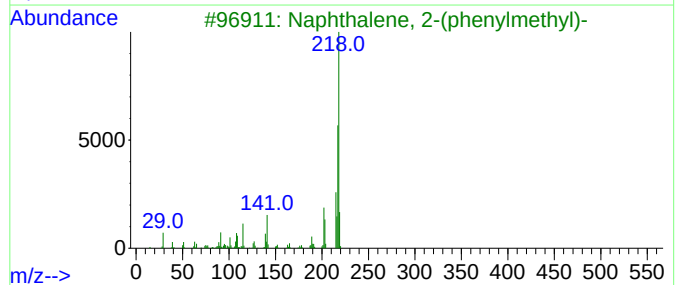
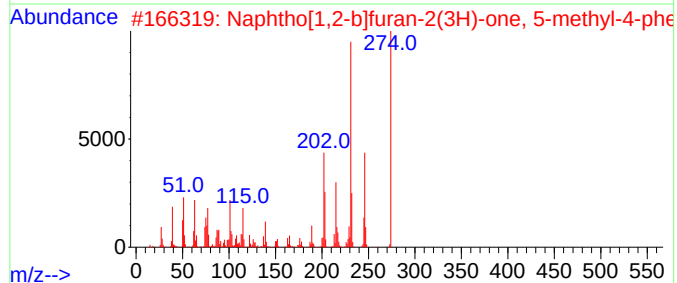
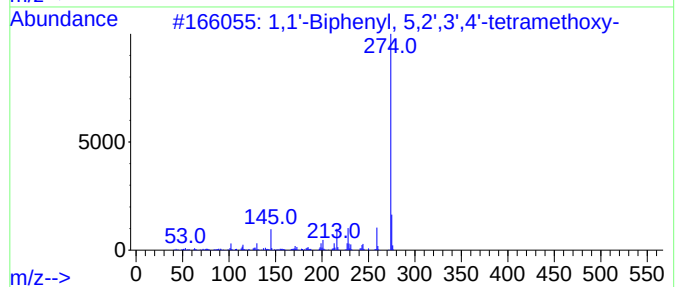
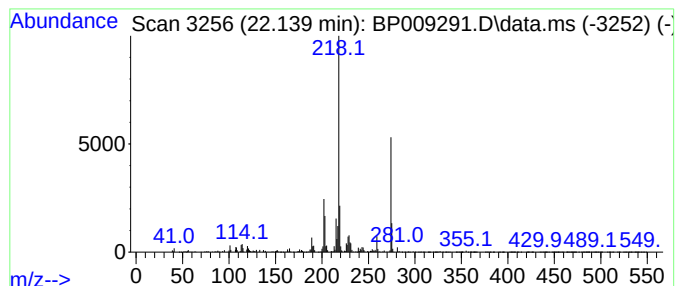
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Peak Number 5 1,1'-Biphenyl, 5,2',3',4'-t... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.139	3.33 ng	1090600	Chrysene-d12	21.321

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,1'-Biphenyl, 5,2',3',4'-tetram...	274	C16H18O4	119101-30-3	56
2			Naphtho[1,2-b]furan-2(3H)-one, 5...	274	C19H14O2	077573-41-2	55
3			Naphthalene, 2-(phenylmethyl)-	218	C17H14	000613-59-2	53
4			3,6-Dibora-2,4,5,7-tetraoxaphena...	274	C12H12B2O6	1000159-66-2	52
5			1H-Cyclopenta[1]phenanthrene, 2,...	218	C17H14	000723-98-8	49



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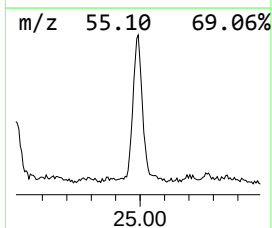
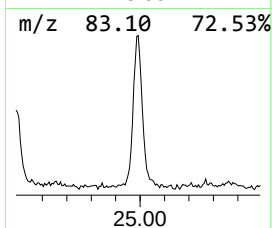
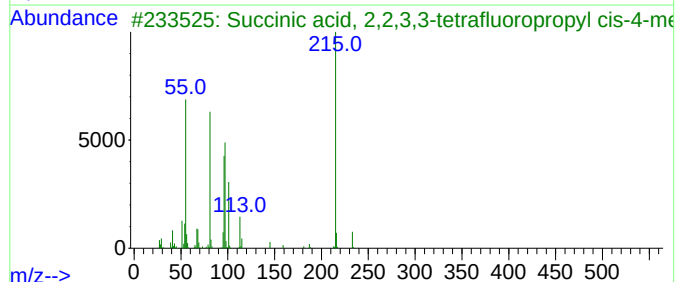
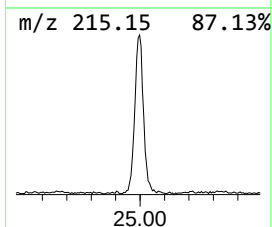
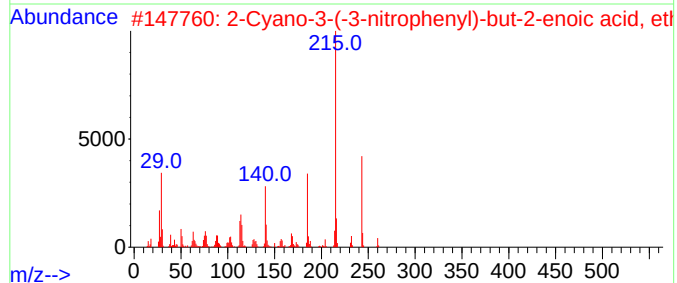
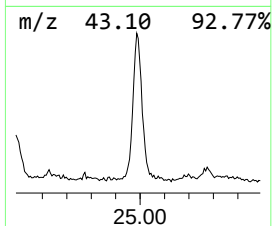
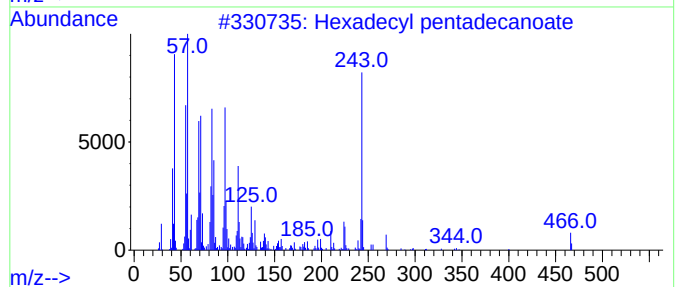
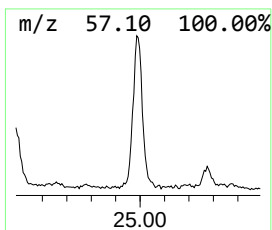
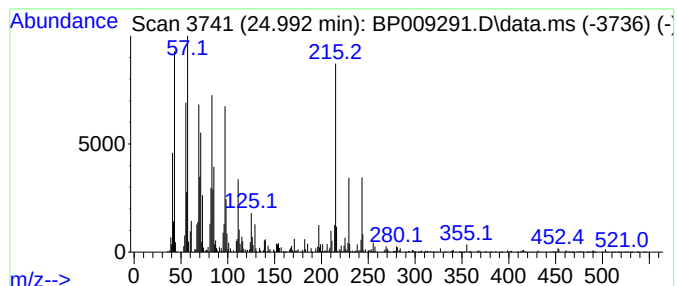
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Peak Number 6 Hexadecyl pentadecanoate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.992	4.24 ng	1373540	Perylene-d12	23.733

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecyl pentadecanoate	466	C31H62O2	036617-33-1	50
2			2-Cyano-3-(-3-nitrophenyl)-but-2...	260	C13H12N2O4	014442-35-4	35
3			Succinic acid, 2,2,3,3-tetraflu...	328	C14H20F4O4	1000390-05-3	32
4			1-Methyl-5-phenylsulfanyl-1H-pyr...	215	C11H9N3S	1000311-79-9	27
5			Kinetin	215	C10H9N5O	000525-79-1	27



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	3.075	11.0	ng	1699920	1	7.822	3082370	20.0
n-Hexadecanoic ...	18.122	2.3	ng	657302	4	17.216	5625260	20.0
1-Heneicosanol	21.051	3.5	ng	1162940	5	21.321	6557870	20.0
1,1'-Biphenyl, ...	22.139	3.3	ng	1090600	5	21.321	6557870	20.0
Hexadecyl penta...	24.992	4.2	ng	1373540	6	23.733	6479440	20.0