

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120123\
 Data File : BF136372.D
 Acq On : 02 Dec 2023 10:59
 Operator : CG\JU
 Sample : 05434-15
 Misc :
 ALS Vial : 43 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 COMP-8

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-BF112723.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF136372.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.151	3	11	18	rVB	286574	403064	13.82%	2.221%
2	5.063	499	506	515	rVB	54698	76146	2.61%	0.420%
3	5.451	567	572	575	rBV	3079427	2793206	95.78%	15.392%
4	6.445	735	741	744	rBV	2447259	2435975	83.53%	13.423%
5	6.804	799	802	806	rBV	766969	613486	21.04%	3.381%
6	7.369	892	898	901	rBV	1584614	1543447	52.92%	8.505%
7	8.081	1014	1019	1023	rBV	764645	654843	22.45%	3.608%
8	9.163	1198	1203	1206	rBV	2831595	2513677	86.19%	13.851%
9	9.563	1269	1271	1274	rVB	50737	39159	1.34%	0.216%
10	9.839	1311	1318	1321	rBV	787329	613437	21.03%	3.380%
11	10.627	1448	1452	1464	rBV	1440413	1410710	48.37%	7.774%
12	10.763	1471	1475	1478	rBV	48141	45598	1.56%	0.251%
13	11.327	1568	1571	1575	rBV	679767	635470	21.79%	3.502%
14	11.868	1659	1663	1673	rBV2	113898	143410	4.92%	0.790%
15	12.433	1753	1759	1763	rBV4	24597	32068	1.10%	0.177%
16	12.545	1775	1778	1782	rBV	22693	32692	1.12%	0.180%
17	12.657	1794	1797	1803	rBV2	34032	43976	1.51%	0.242%
18	12.927	1839	1843	1847	rBV	3090939	2916400	100.00%	16.070%
19	13.168	1881	1884	1887	rBV2	33762	33860	1.16%	0.187%
20	13.839	1996	1998	2002	rBV	32486	31565	1.08%	0.174%
21	13.927	2008	2013	2018	rBV9	38487	105480	3.62%	0.581%
22	13.986	2019	2023	2026	rVV	626771	595763	20.43%	3.283%
23	14.468	2102	2105	2108	rBV2	50840	52634	1.80%	0.290%
24	15.468	2271	2275	2282	rBV	312925	381606	13.08%	2.103%

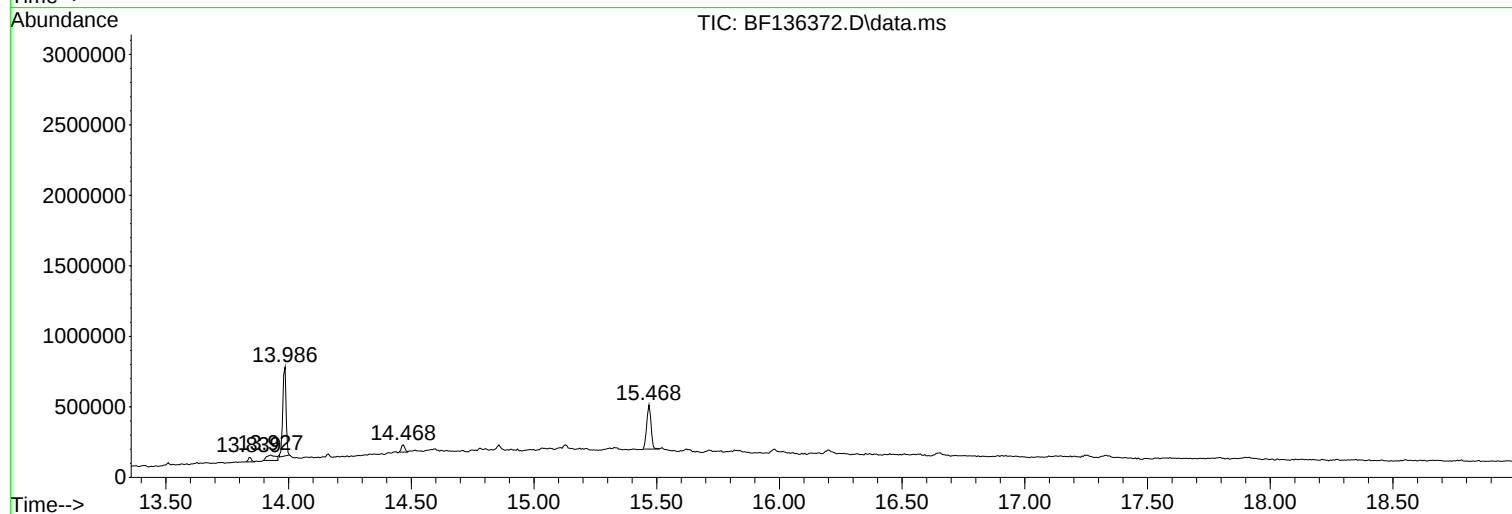
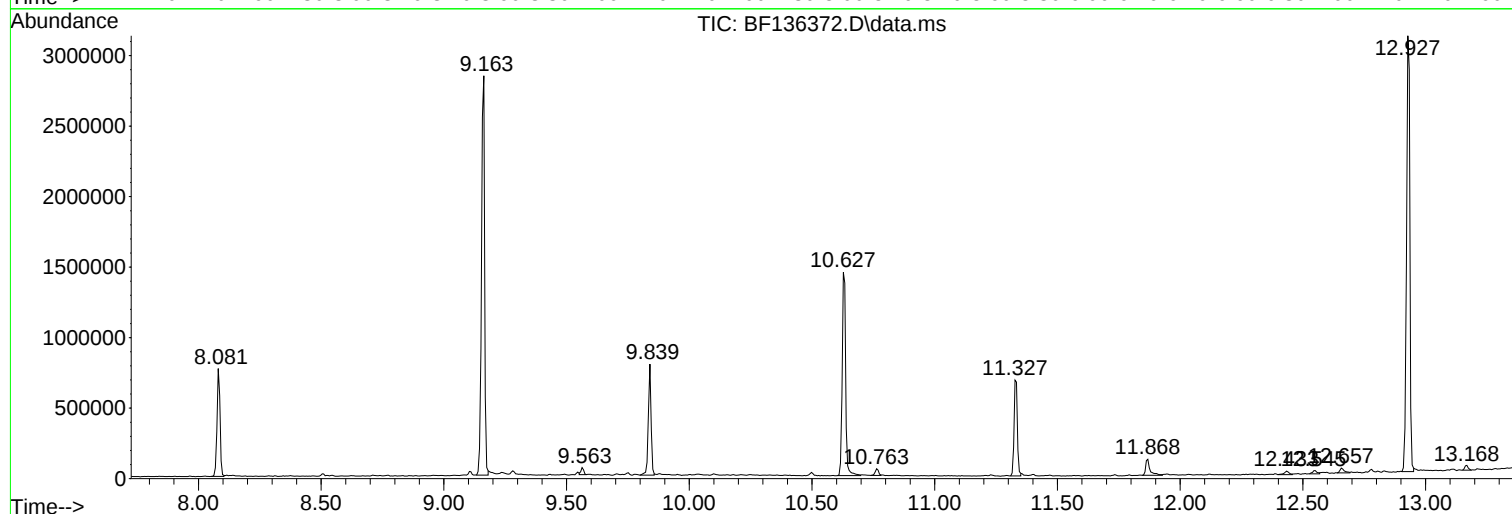
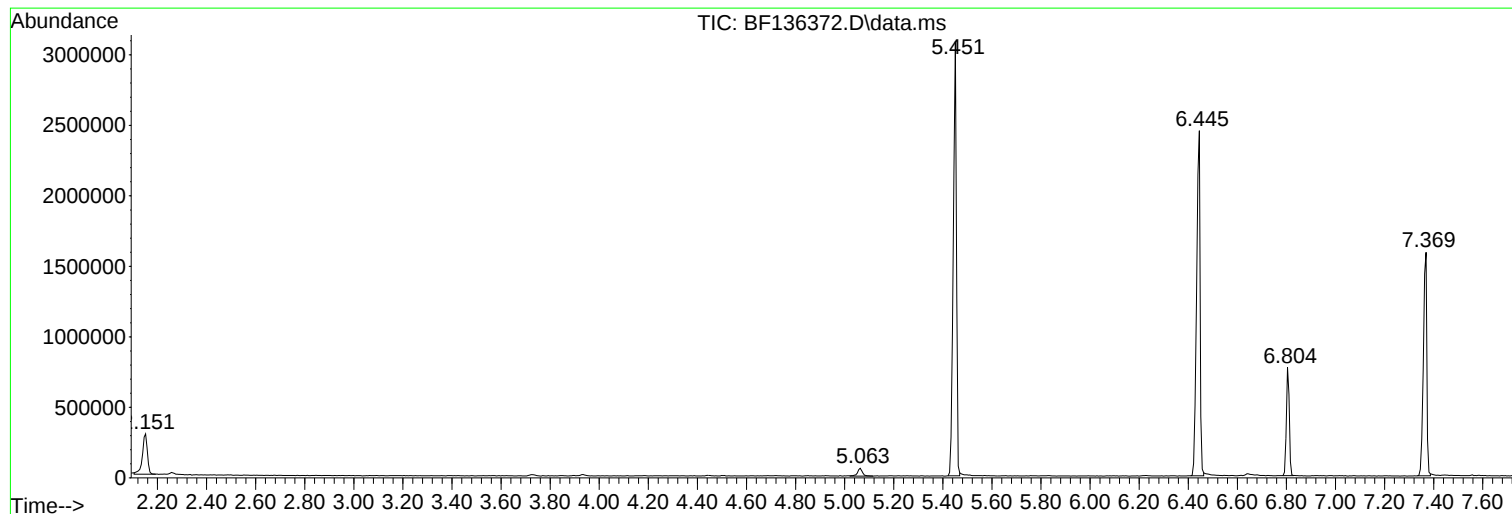
Sum of corrected areas: 18147672

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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112723.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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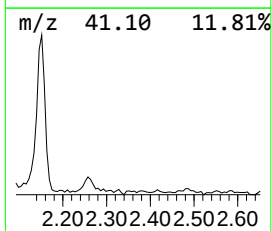
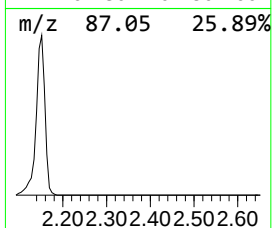
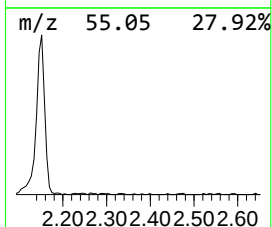
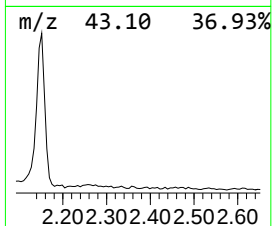
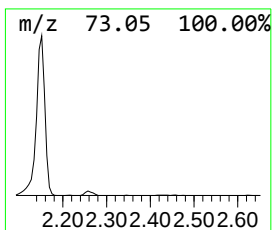
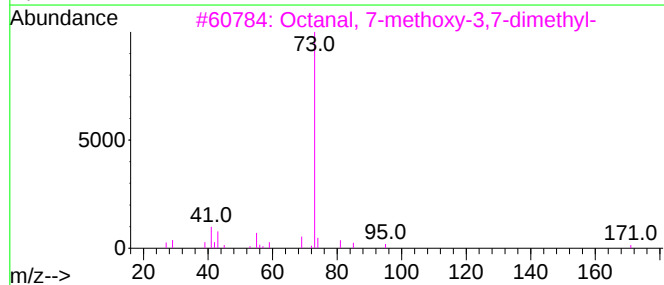
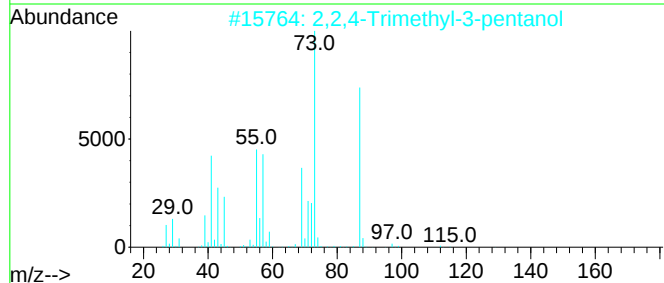
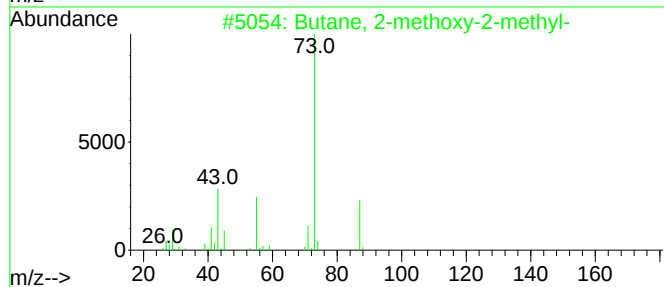
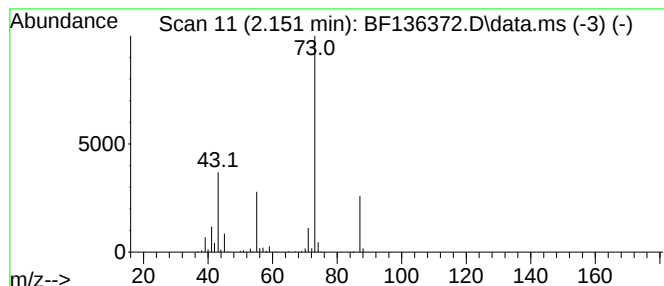
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.151	13.14 ng	403064	1,4-Dichlorobenzene-d4	6.804

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3			Octanal, 7-methoxy-3,7-dimethyl-	186	C11H22O2	003613-30-7	25
4			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
5			1-(2-Methoxyethoxy)-2-methyl-2-p...	162	C8H18O3	1000364-24-4	23



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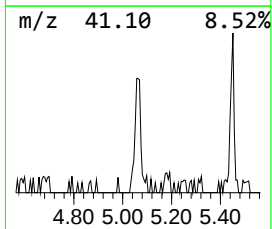
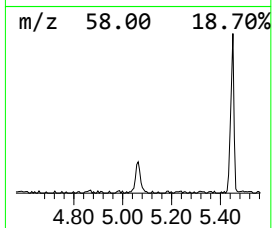
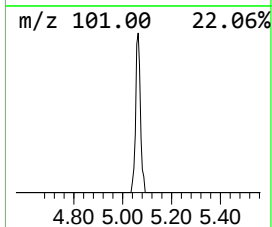
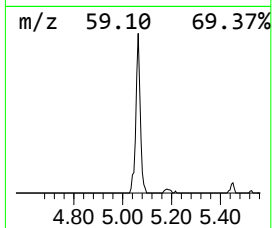
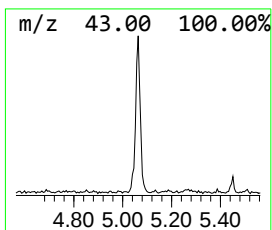
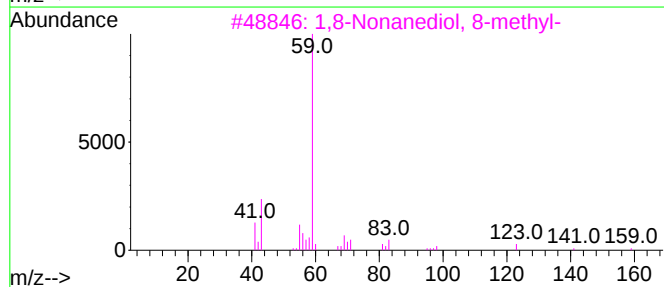
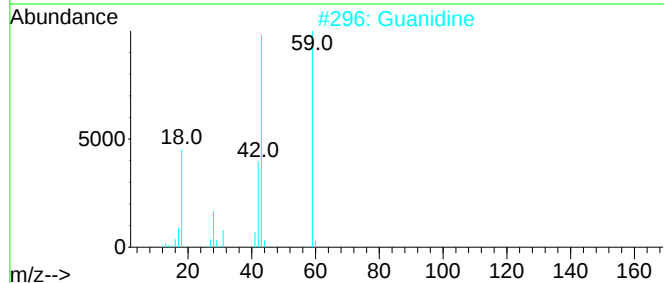
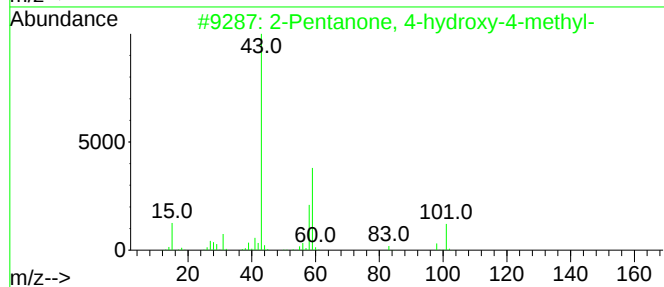
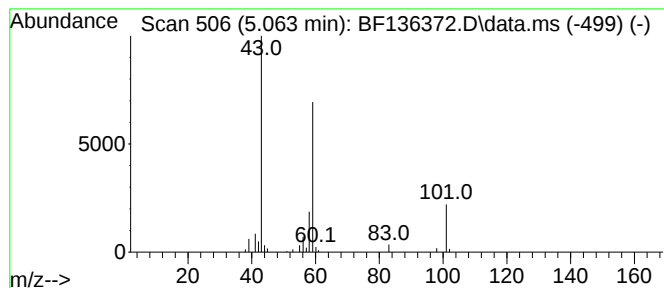
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.063	2.48 ng	76146	1,4-Dichlorobenzene-d4	6.804

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		Guanidine	59	CH5N3	000113-00-8	43
3		1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	25
4		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	25
5		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25



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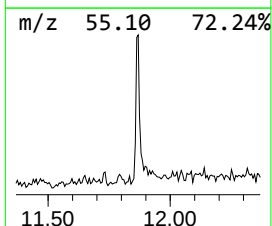
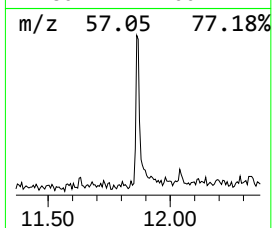
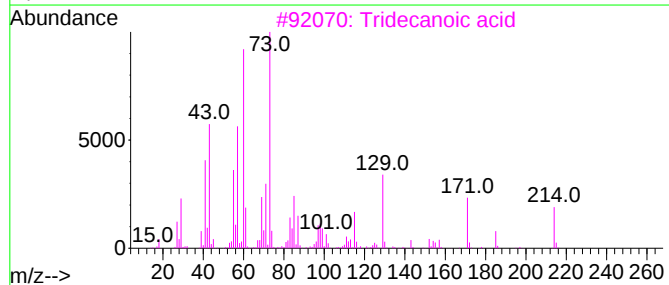
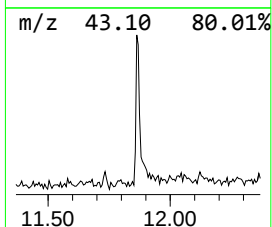
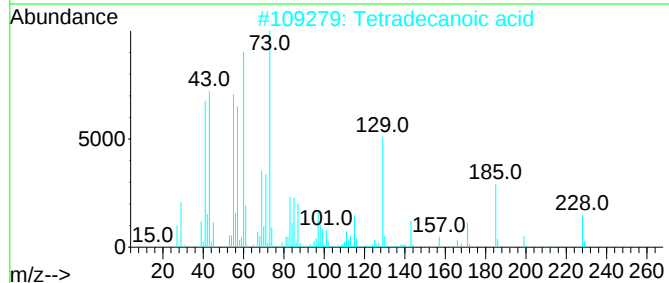
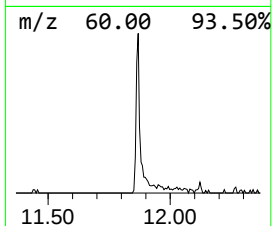
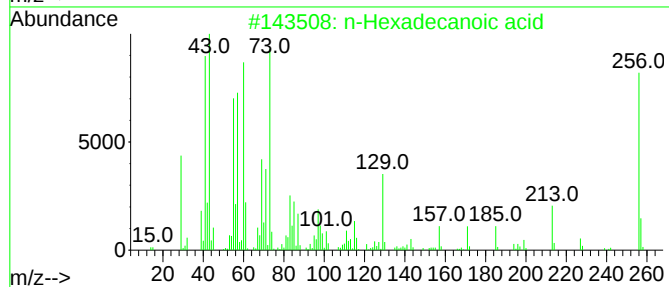
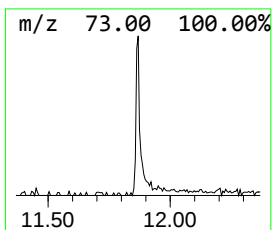
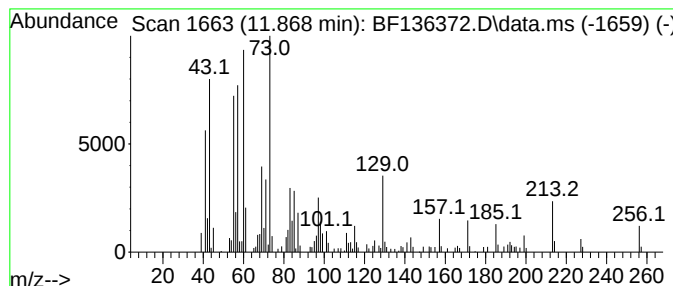
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.868	4.51 ng	143410	Phenanthrene-d10	11.333	
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	92
3	Tridecanoic acid	214	C13H26O2	000638-53-9	90
4	Undecanoic acid	186	C11H22O2	000112-37-8	70
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	68



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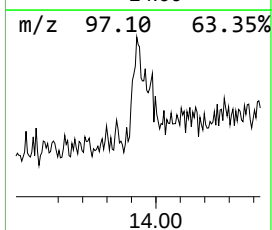
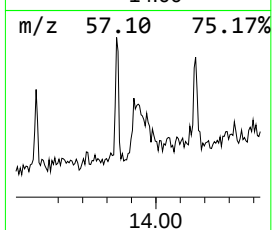
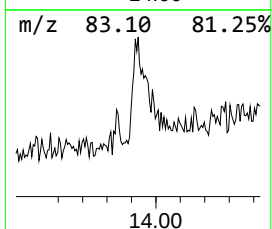
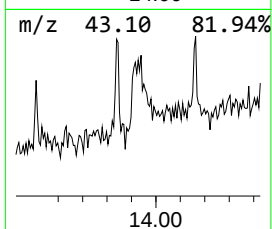
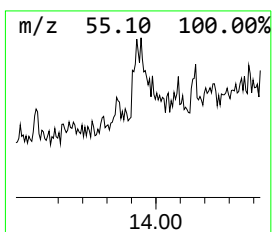
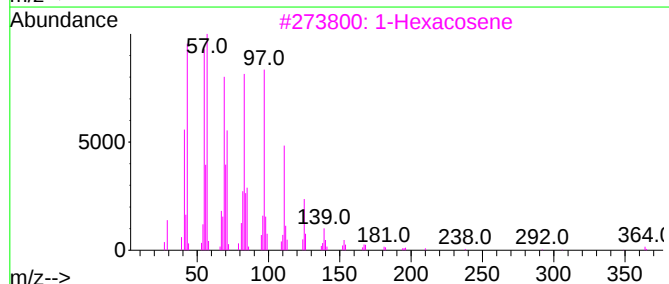
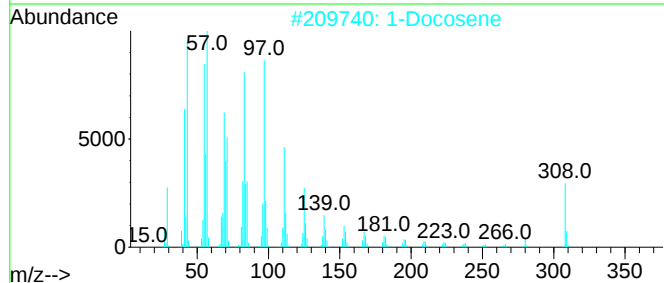
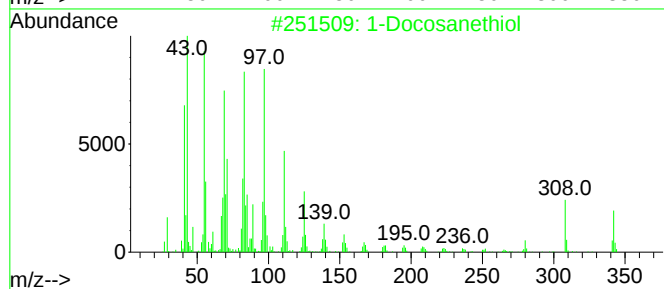
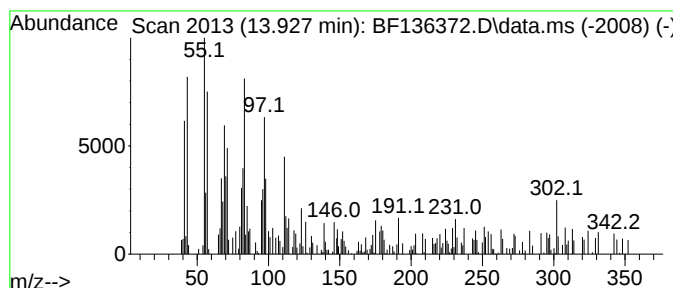
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Peak Number 4 1-Docosanethiol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.927	3.54 ng	105480	Chrysene-d12	13.986	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosanethiol	342	C22H46S	007773-83-3	89
2	1-Docosene	308	C22H44	001599-67-3	70
3	1-Hexacosene	364	C26H52	018835-33-1	64
4	Behenic alcohol	326	C22H46O	000661-19-8	58
5	1-Octadecene	252	C18H36	000112-88-9	58



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.151	13.1	ng	403064	1	6.804	613486	20.0
2-Pentanone, 4-...	5.063	2.5	ng	76146	1	6.804	613486	20.0
n-Hexadecanoic ...	11.868	4.5	ng	143410	4	11.333	635470	20.0
1-Docosanethiol	13.927	3.5	ng	105480	5	13.986	595763	20.0