

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM080223\
 Data File : BM041244.D
 Acq On : 02 Aug 2023 14:38
 Operator : MA/JU
 Sample : 03810-03
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 B-P16A

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_M\Methods\8270-BM072823.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM041244.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.369	364	371	386	rBV	1873055	2741562	48.48%	6.773%
2	6.451	549	555	564	rVB	53778	82566	1.46%	0.204%
3	6.981	638	645	660	rBV	1930769	3042327	53.80%	7.516%
4	7.410	712	718	727	rBV2	29347	65525	1.16%	0.162%
5	7.798	772	784	791	rBV	677122	1069160	18.91%	2.641%
6	8.975	975	984	999	rBV	1168207	1931669	34.16%	4.772%
7	10.604	1254	1261	1269	rBV	967938	1583627	28.00%	3.912%
8	13.080	1675	1682	1694	rBV	3255015	4559654	80.63%	11.264%
9	13.351	1719	1728	1733	rVB	47902	86089	1.52%	0.213%
10	13.763	1793	1798	1806	rBV	94324	138617	2.45%	0.342%
11	14.439	1903	1913	1914	rBV	801634	1051185	18.59%	2.597%
12	14.463	1914	1917	1923	rVB	1566618	2219122	39.24%	5.482%
13	14.704	1952	1958	1967	rBV	196178	315341	5.58%	0.779%
14	14.886	1979	1989	1992	rBV6	29477	56782	1.00%	0.140%
15	15.215	2039	2045	2050	rBV	71571	96819	1.71%	0.239%
16	15.345	2062	2067	2081	rVB	63671	93677	1.66%	0.231%
17	15.904	2158	2162	2165	rBV	57358	86575	1.53%	0.214%
18	15.968	2167	2173	2180	rVV	2805215	4017437	71.04%	9.925%
19	16.033	2180	2184	2190	rVB	81972	119567	2.11%	0.295%
20	17.221	2377	2386	2398	rBV	1906951	2805827	49.62%	6.932%
21	18.009	2515	2520	2525	rBV4	40439	69863	1.24%	0.173%
22	18.068	2525	2530	2535	rBV2	244722	437402	7.73%	1.081%
23	18.127	2535	2540	2549	rVB	1088202	1556698	27.53%	3.846%
24	18.721	2637	2641	2647	rBV	185231	247807	4.38%	0.612%
25	19.162	2713	2716	2721	rBV2	58612	85684	1.52%	0.212%
26	19.292	2734	2738	2750	rVB	160309	329610	5.83%	0.814%
27	19.409	2754	2758	2766	rVV	377641	594787	10.52%	1.469%
28	19.480	2766	2770	2776	rVB	109011	161334	2.85%	0.399%
29	19.656	2797	2800	2809	rVB	126406	202000	3.57%	0.499%
30	19.862	2830	2835	2840	rBV	4980760	5655148	100.00%	13.971%
31	21.133	3048	3051	3060	rVB	466947	626914	11.09%	1.549%
32	21.427	3096	3101	3106	rBV	1812986	2323271	41.08%	5.740%
33	23.803	3499	3505	3513	rVB	1085952	2024731	35.80%	5.002%

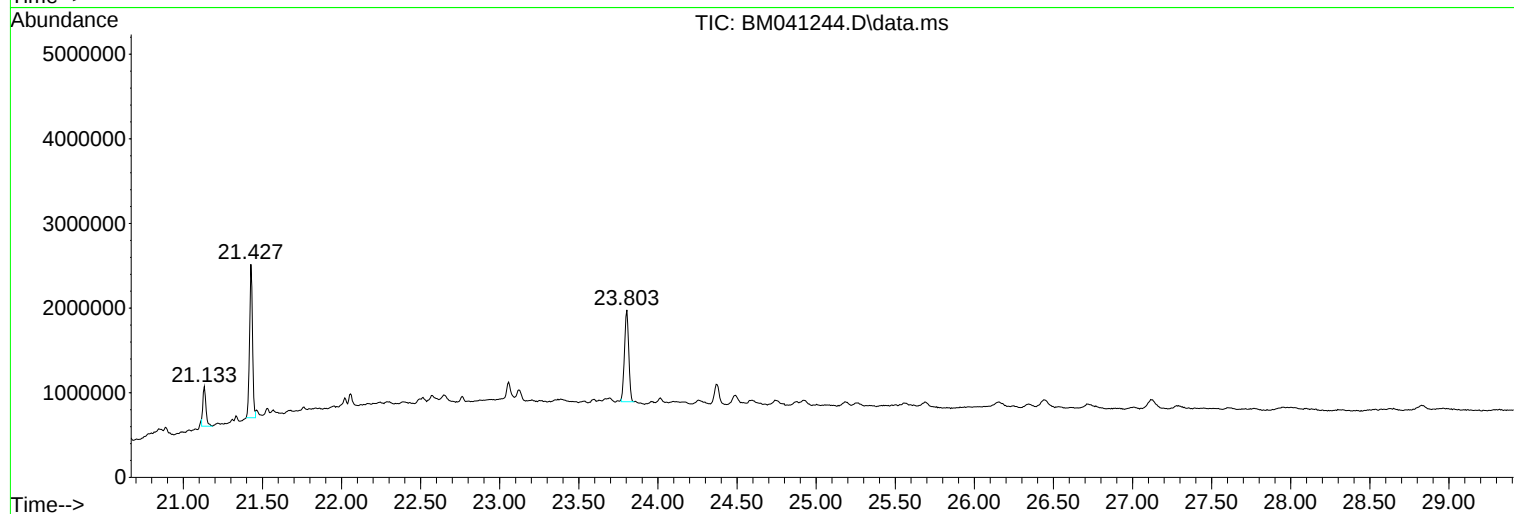
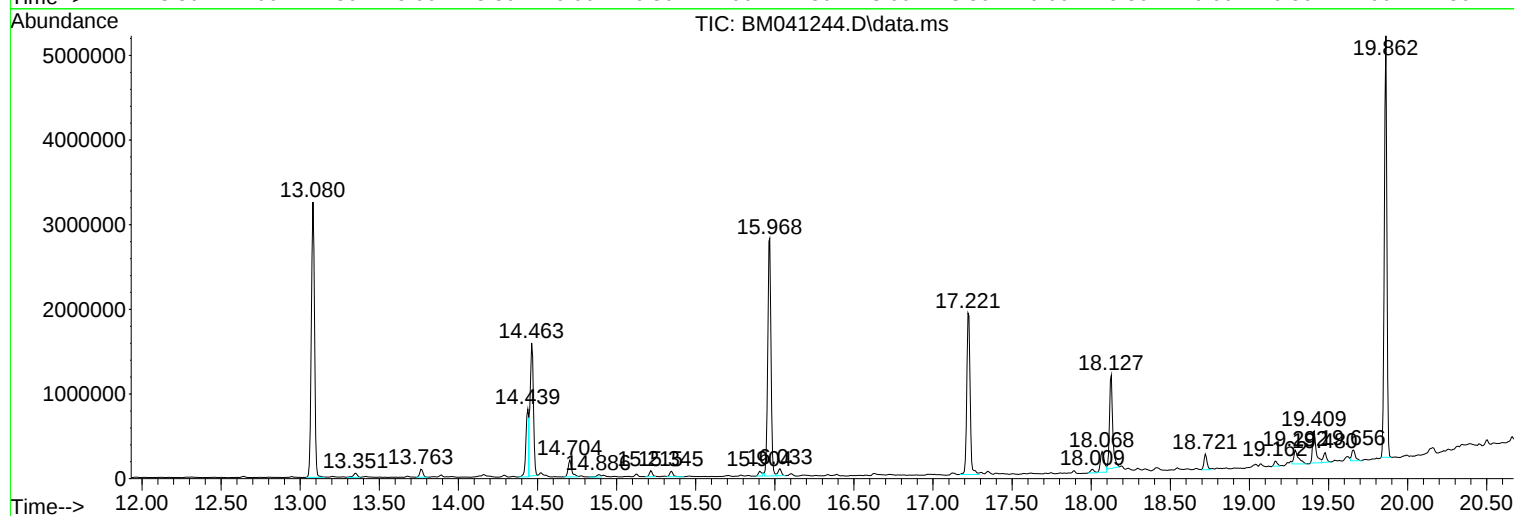
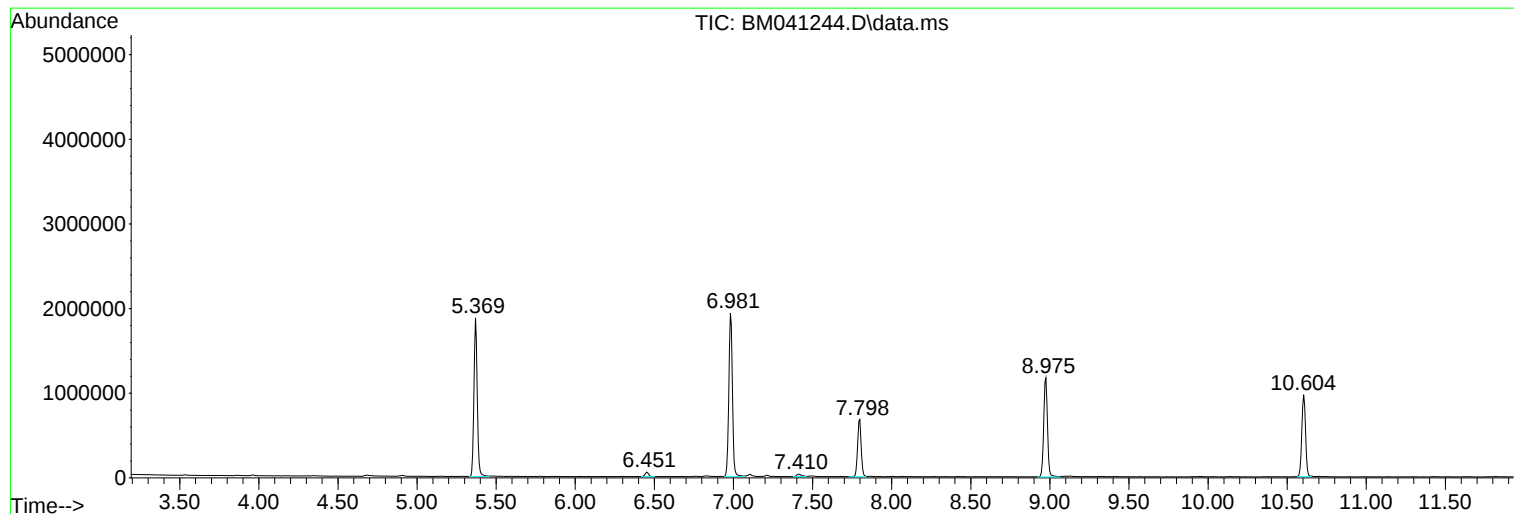
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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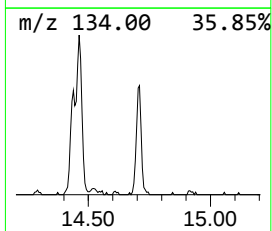
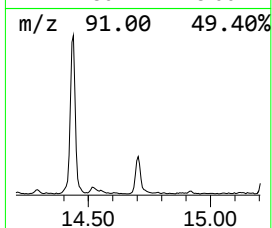
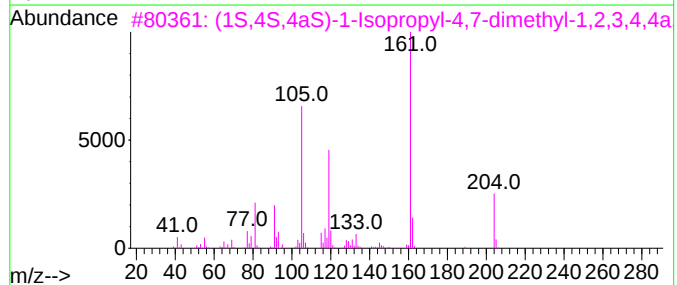
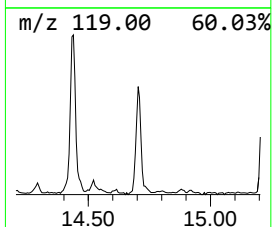
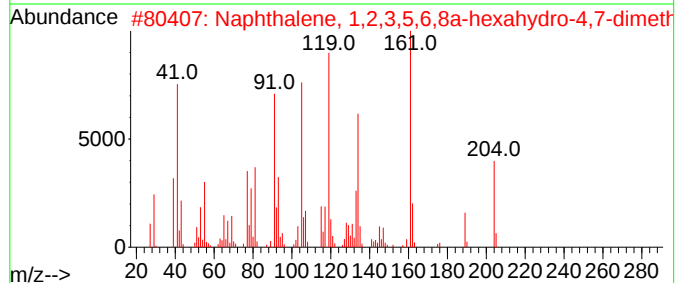
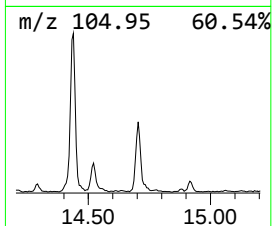
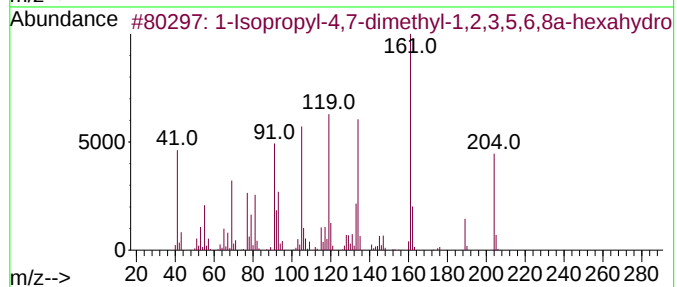
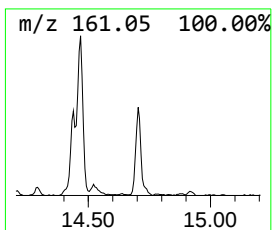
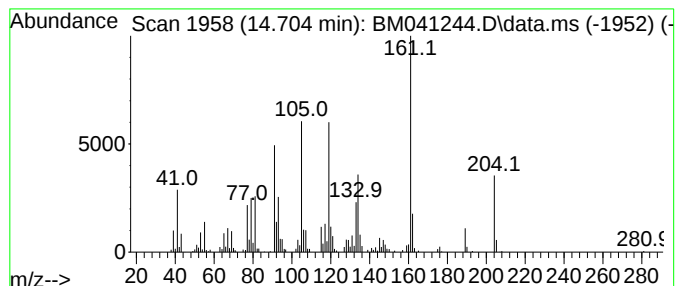
Instrument :
BNA_M
ClientSampleId :
B-P16A

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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 1-Isopropyl-4,7-dimethyl-1,... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.704	2.84 ng	315341	Acenaphthene-d10	14.463	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Isopropyl-4,7-dimethyl-1,2,3,5...	204	C15H24	016729-01-4	96
2	Naphthalene, 1,2,3,5,6,8a-hexahy...	204	C15H24	000483-76-1	96
3	(1S,4S,4aS)-1-Isopropyl-4,7-dime...	204	C15H24	267665-20-3	94
4	Copaene	204	C15H24	003856-25-5	94
5	.gamma.-Muurolene	204	C15H24	030021-74-0	93



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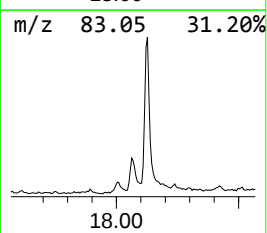
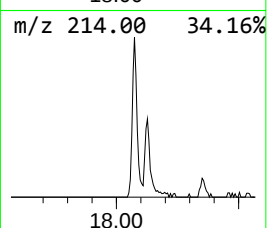
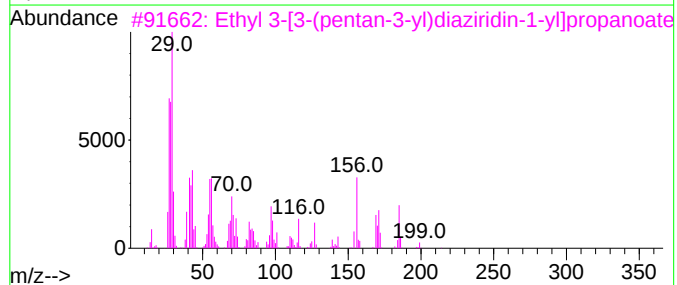
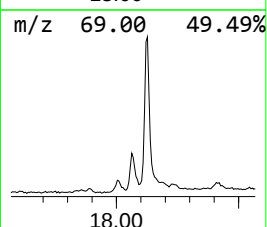
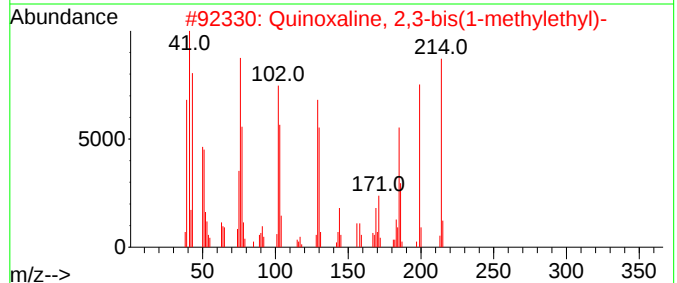
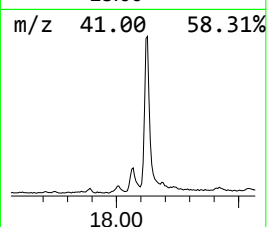
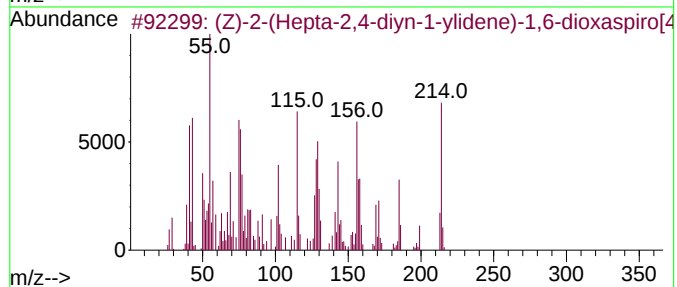
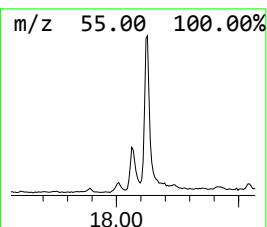
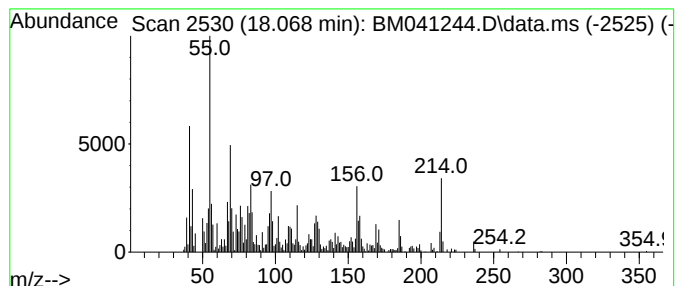
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Peak Number 2 unknown18.068 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.068	3.12 ng	437402	Phenanthrene-d10	17.221

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	(Z)-2-(Hepta-2,4-diyn-1-ylidene)...	214	C14H14O2	206062-16-0	43		
2	Quinoxaline, 2,3-bis(1-methyleth...	214	C14H18N2	077611-56-4	27		
3	Ethyl 3-[3-(pentan-3-yl)diazirid...	214	C11H22N2O2	1000444-79-9	14		
4	Dodecylsuccinic anhydride	268	C16H28O3	002561-85-5	12		
5	Hexadecenoic acid, Z-11-	254	C16H30O2	002416-20-8	11		



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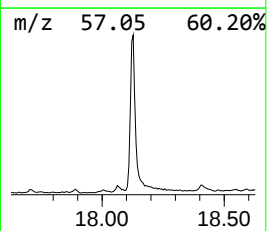
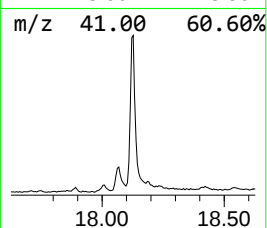
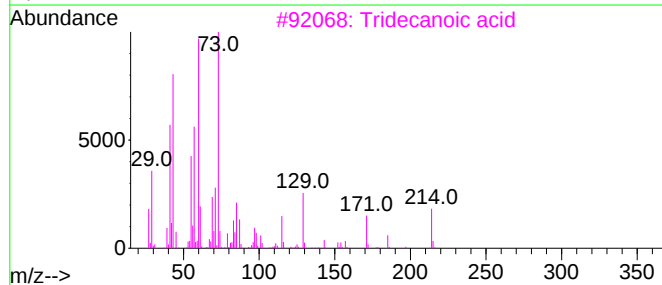
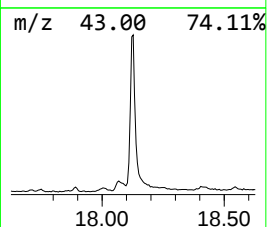
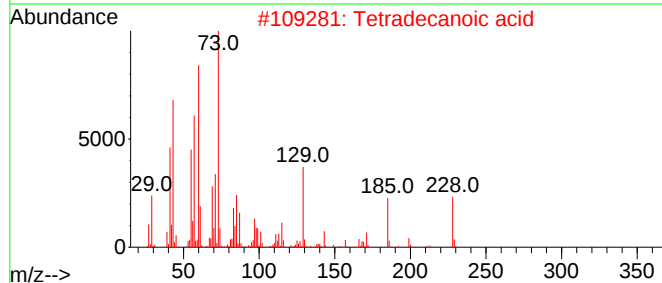
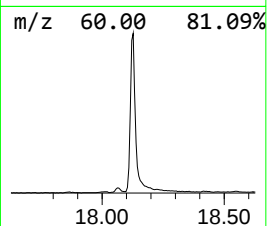
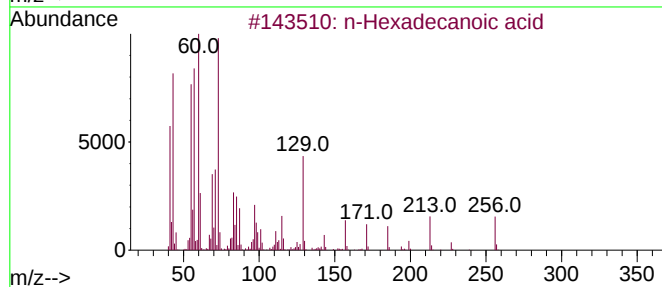
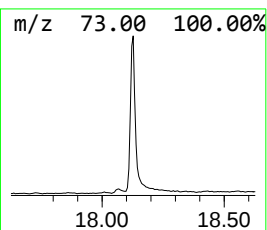
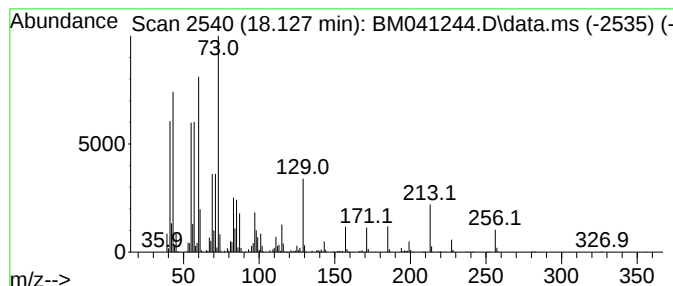
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.127	11.10 ng	1556700	Phenanthrene-d10	17.221

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	94
3			Tridecanoic acid	214	C13H26O2	000638-53-9	90
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	81
5			Octadecanoic acid	284	C18H36O2	000057-11-4	49



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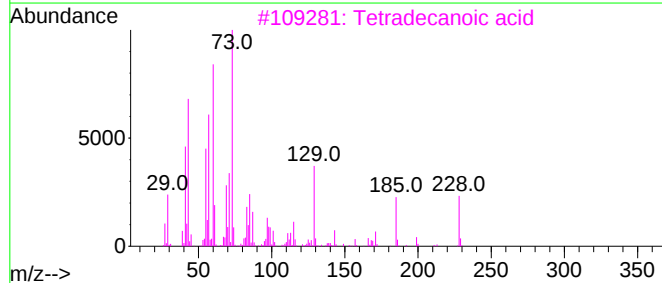
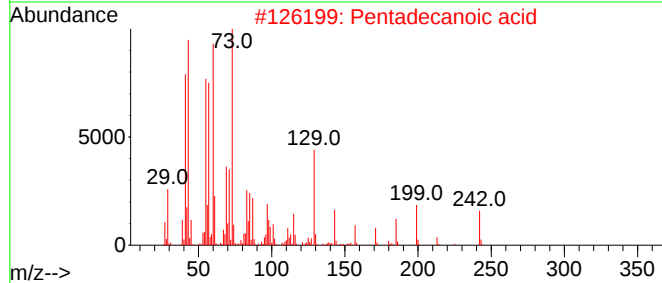
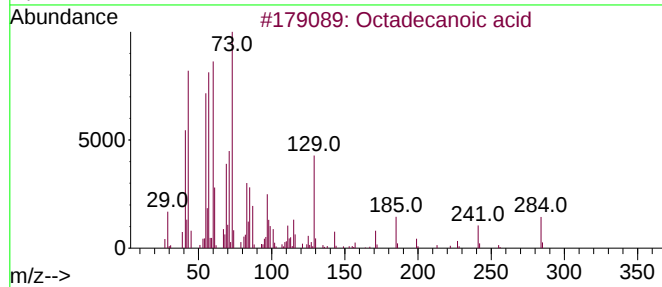
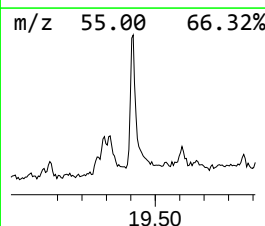
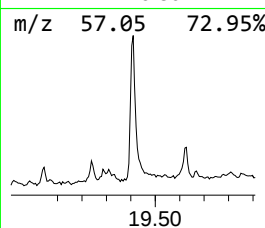
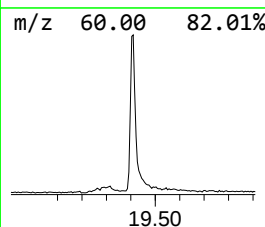
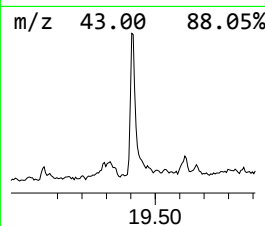
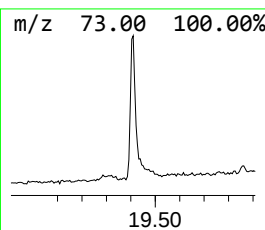
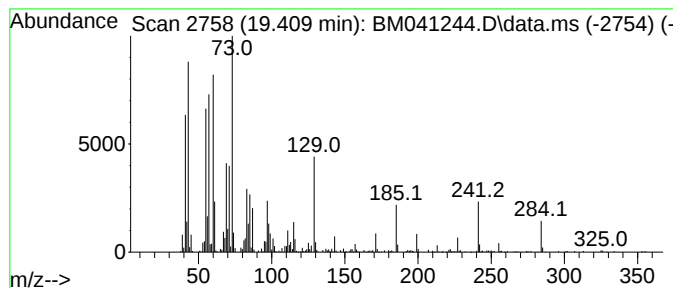
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Peak Number 5 Octadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.409	5.12 ng	594787	Chrysene-d12	21.427

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	93
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	87
4			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	83
5			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	72



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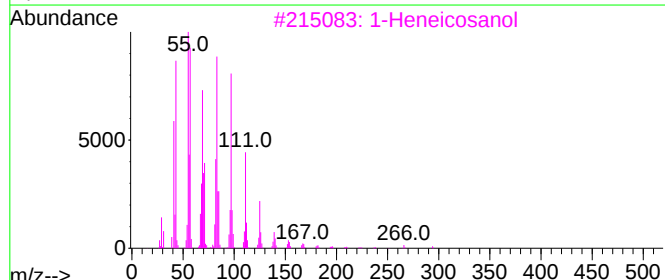
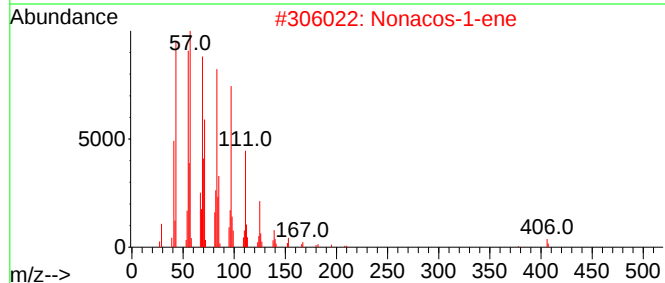
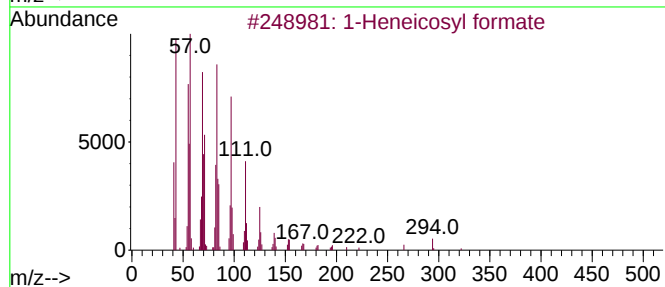
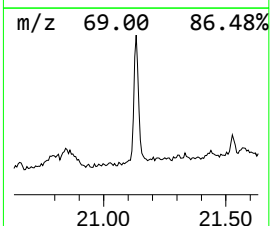
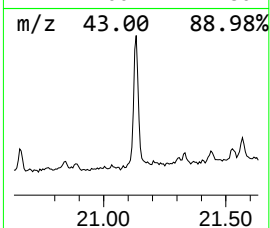
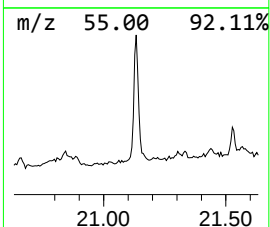
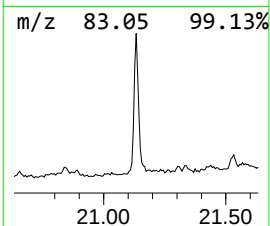
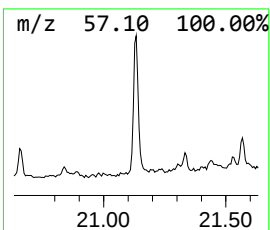
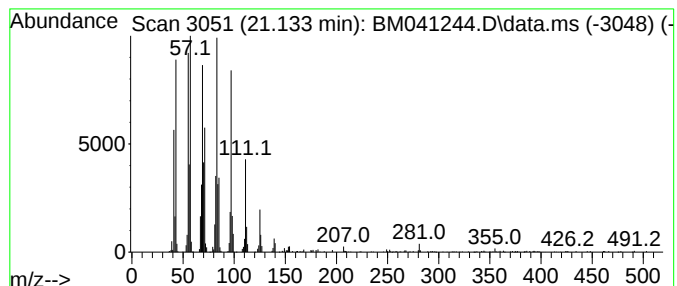
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Peak Number 6 1-Heneicosyl formate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.133	5.40 ng	626914	Chrysene-d12	21.427

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Heneicosyl formate	340	C22H44O2	077899-03-7	97
2			Nonacos-1-ene	406	C29H58	018835-35-3	94
3			1-Heneicosanol	312	C21H44O	015594-90-8	94
4			Behenic alcohol	326	C22H46O	000661-19-8	94
5			2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	94



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Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
B-P16A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM072823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
1-Isopropyl-4,7...	14.704	2.8	ng	315341	3	14.463	2219120	20.0
unknown18.068	18.068	3.1	ng	437402	4	17.221	2805830	20.0
n-Hexadecanoic ...	18.127	11.1	ng	1556700	4	17.221	2805830	20.0
Octadecanoic acid	19.409	5.1	ng	594787	5	21.427	2323270	20.0
1-Heneicosyl fo...	21.133	5.4	ng	626914	5	21.427	2323270	20.0