

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM082024\
 Data File : BM047288.D
 Acq On : 21 Aug 2024 02:52
 Operator : RC/JU
 Sample : P3580-01
 Misc :
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 926-K1-SD-0-0.5-081224

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-BM081024.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM047288.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.269	62	65	79	rVB	55384	96500	1.64%	0.185%
2	4.569	280	286	294	rBV	193944	263327	4.47%	0.504%
3	5.016	356	362	375	rBV	2954824	4174092	70.91%	7.985%
4	6.575	616	627	643	rBV	2651857	4233002	71.91%	8.098%
5	6.992	694	698	708	rBV	37729	74968	1.27%	0.143%
6	7.357	752	760	769	rBV	1194260	1819887	30.92%	3.481%
7	7.657	805	811	818	rVB	90748	132425	2.25%	0.253%
8	8.504	945	955	966	rBV	1772016	2889231	49.08%	5.527%
9	10.110	1220	1228	1235	rBV	1385396	2302439	39.12%	4.405%
10	10.880	1352	1359	1372	rBV	49275	120949	2.05%	0.231%
11	12.621	1647	1655	1673	rBV	3919347	5874763	99.81%	11.238%
12	13.904	1869	1873	1882	rBV5	20833	61523	1.05%	0.118%
13	14.015	1885	1892	1899	rVV	1947784	2771554	47.09%	5.302%
14	14.080	1899	1903	1911	rVB	61777	108409	1.84%	0.207%
15	14.268	1927	1935	1940	rBV3	59149	137918	2.34%	0.264%
16	15.080	2070	2073	2078	rVB	42342	60111	1.02%	0.115%
17	15.527	2137	2149	2160	rBV	2646097	4150743	70.52%	7.940%
18	16.780	2356	2362	2366	rBV	1967496	2829140	48.06%	5.412%
19	16.821	2366	2369	2378	rVV	370747	519790	8.83%	0.994%
20	16.909	2380	2384	2391	rVB	78014	126769	2.15%	0.243%
21	16.986	2392	2397	2405	rBV4	38092	70301	1.19%	0.134%
22	17.198	2425	2433	2443	rBV2	48945	118623	2.02%	0.227%
23	17.715	2517	2521	2528	rVB3	257783	349654	5.94%	0.669%
24	17.851	2540	2544	2549	rVB3	58052	80338	1.36%	0.154%
25	18.856	2709	2715	2724	rBV	711437	974274	16.55%	1.864%
26	19.015	2738	2742	2748	rBV	129289	193861	3.29%	0.371%
27	19.221	2769	2777	2783	rBV	523733	849803	14.44%	1.626%
28	19.280	2783	2787	2797	rVB3	61579	154331	2.62%	0.295%
29	19.445	2807	2815	2826	rBV	4686516	5886226	100.00%	11.260%
30	19.733	2861	2864	2868	rVB2	65231	70989	1.21%	0.136%
31	19.833	2878	2881	2883	rBV2	83394	100292	1.70%	0.192%
32	19.868	2883	2887	2894	rVB	482753	599907	10.19%	1.148%
33	20.309	2957	2962	2968	rVB	1720918	1998825	33.96%	3.824%
34	20.650	3017	3020	3024	rBV	89238	125141	2.13%	0.239%
35	20.756	3034	3038	3044	rBV4	238156	311286	5.29%	0.595%
36	21.015	3076	3082	3087	rBV	2124243	3068959	52.14%	5.871%

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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-BM081024.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	21.056	3087	3089	3099	rVB	276776	348693	5.92%	0.667%
38	21.750	3203	3207	3217	rVB2	301437	645012	10.96%	1.234%
39	22.980	3412	3416	3422	rVB	321798	562635	9.56%	1.076%
40	23.715	3533	3541	3556	rVB	1221070	3017712	51.27%	5.773%

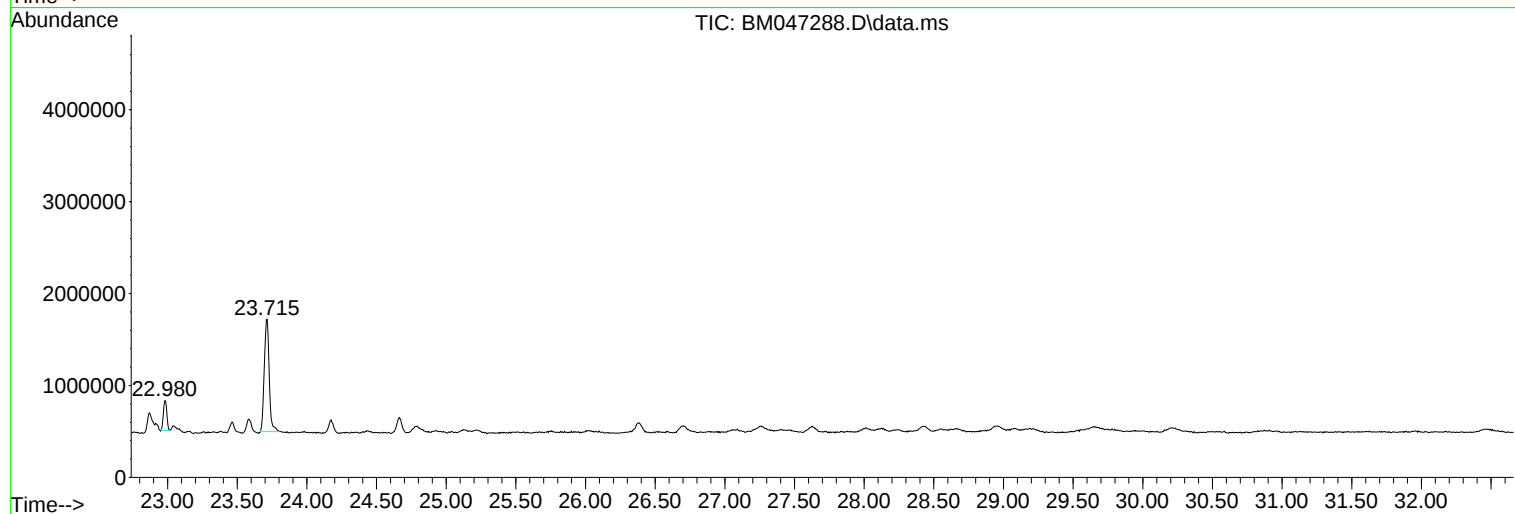
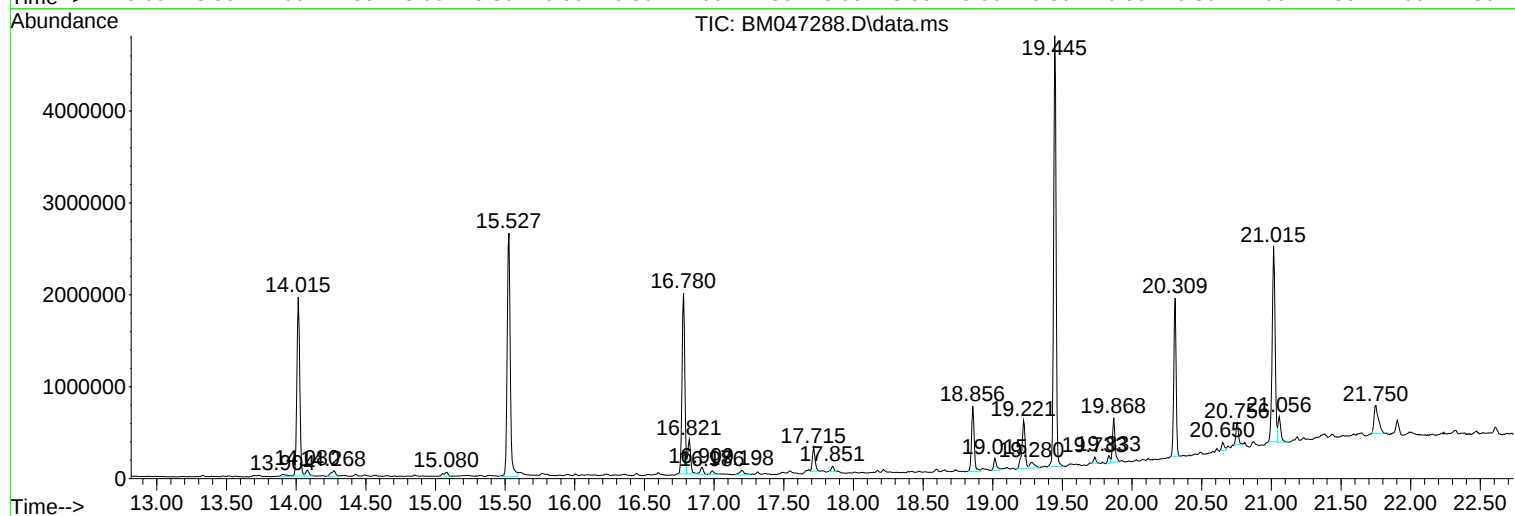
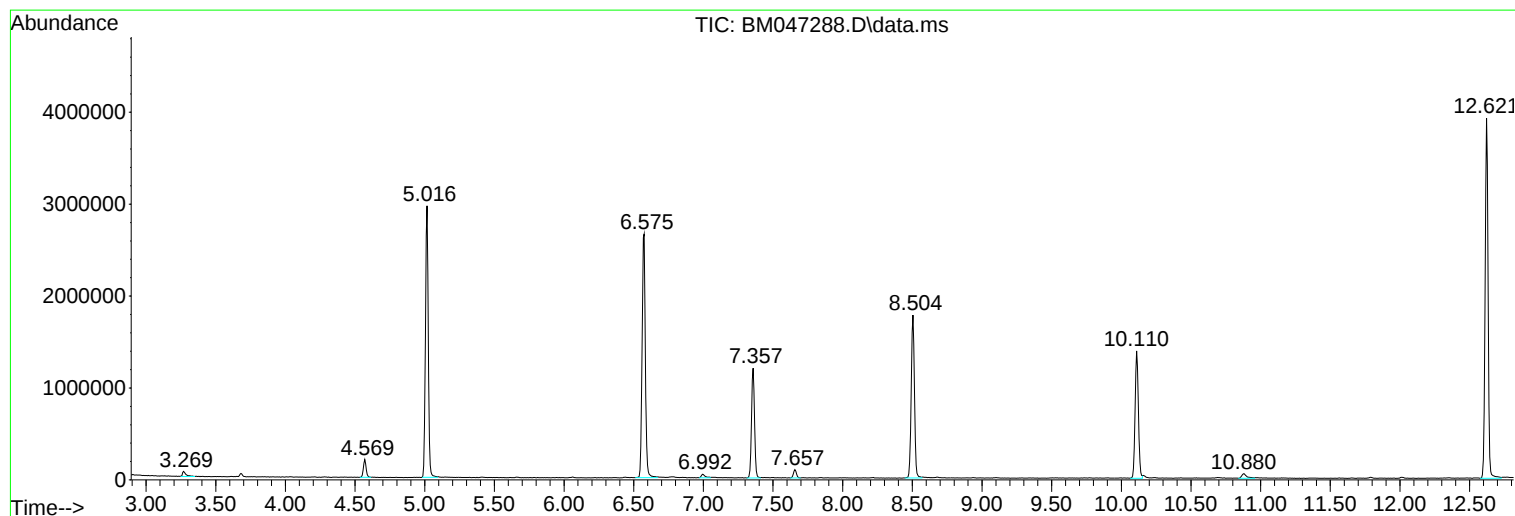
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM081024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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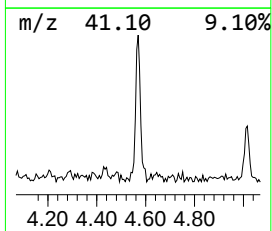
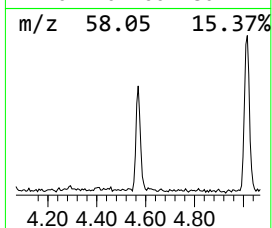
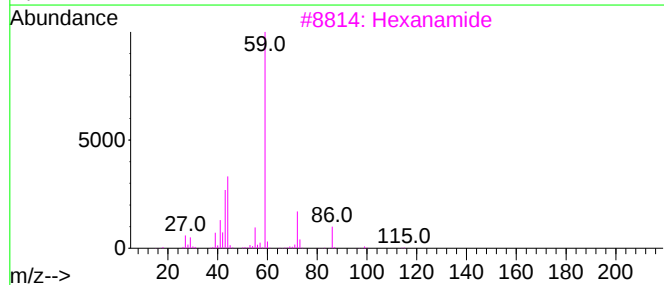
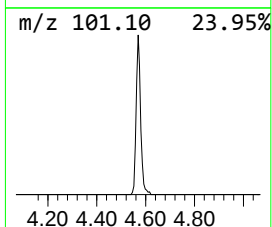
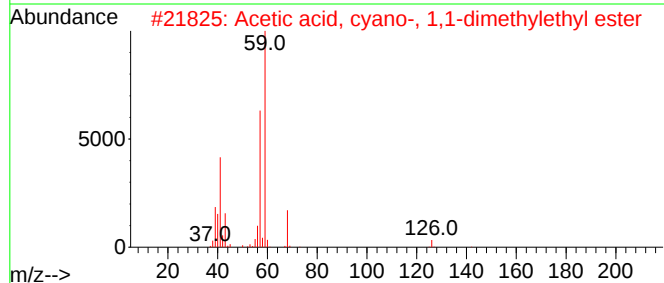
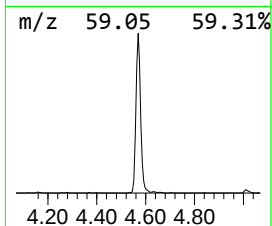
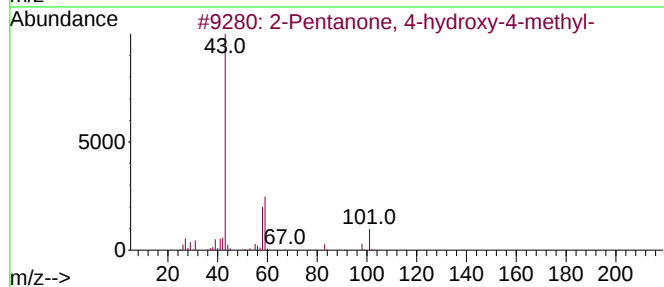
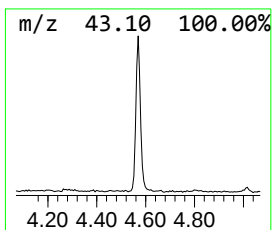
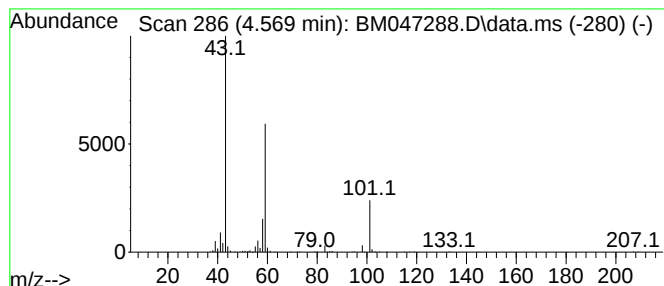
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.569	2.89 ng	263327	1,4-Dichlorobenzene-d4	7.357

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64		
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25		
3	Hexanamide	115	C6H13NO	000628-02-4	16		
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10		
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9		



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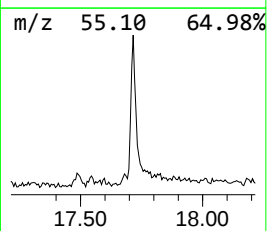
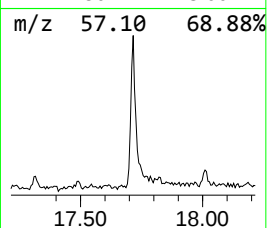
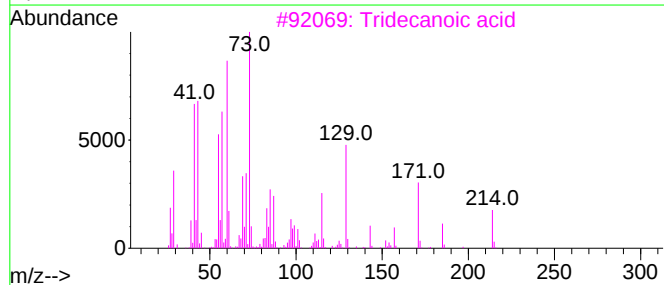
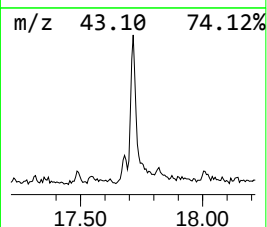
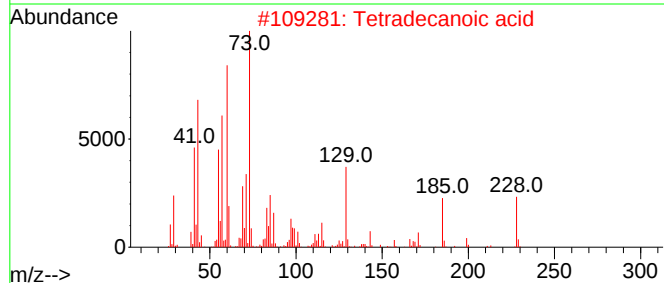
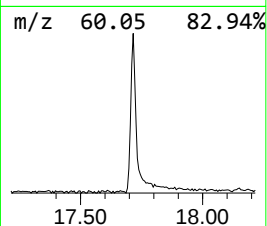
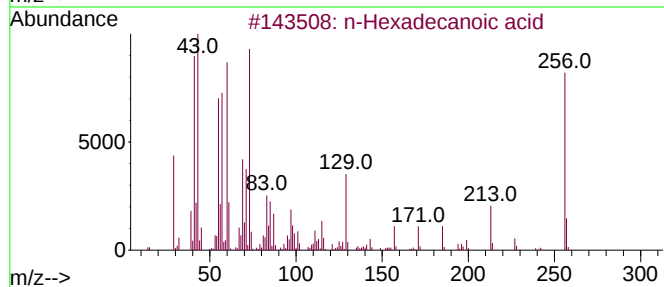
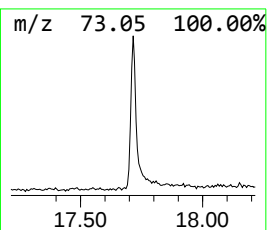
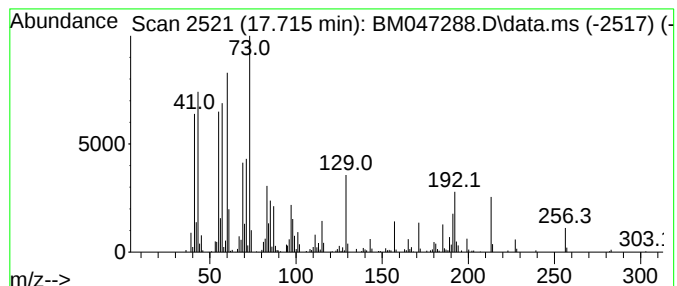
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.715	2.47 ng	349654	Phenanthrene-d10	16.780

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	91
4			Octadecanoic acid	284	C18H36O2	000057-11-4	81
5			Pentadecanoic acid	242	C15H30O2	001002-84-2	76



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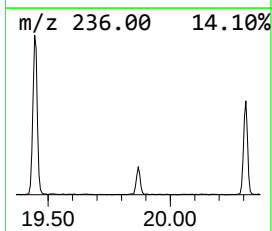
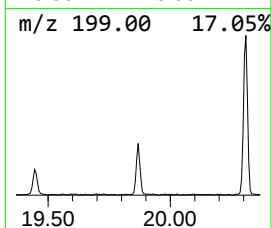
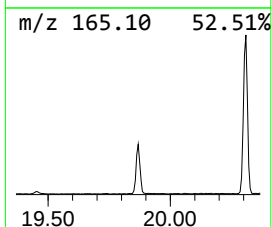
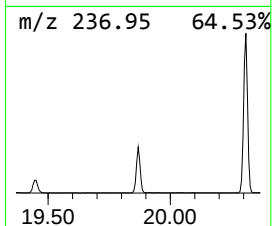
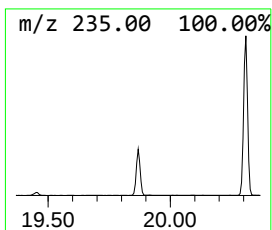
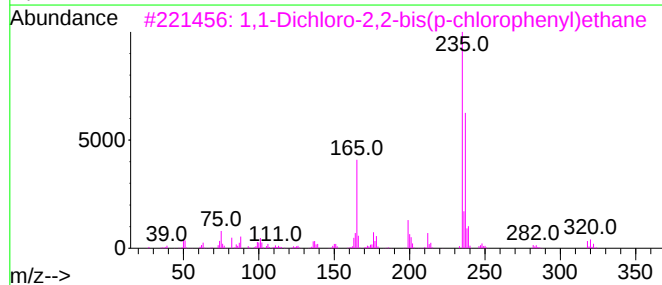
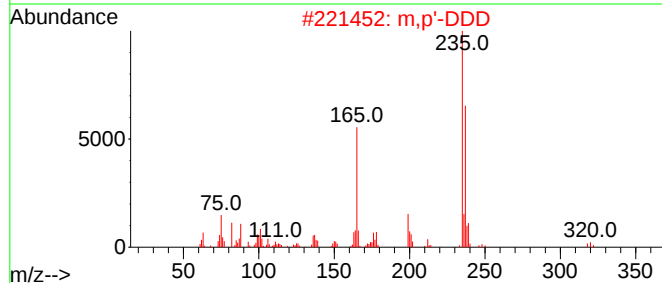
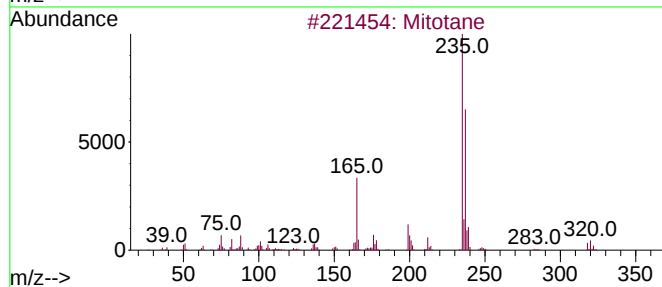
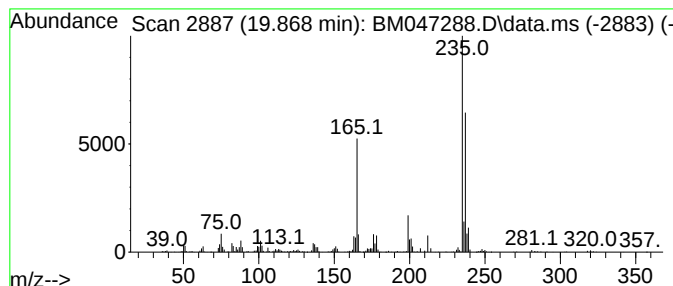
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Mitotane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.868	3.91 ng	599907	Chrysene-d12	21.015

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Mitotane	318	C14H10Cl4	000053-19-0	98
2			m,p'-DDD	318	C14H10Cl4	004329-12-8	95
3			1,1-Dichloro-2,2-bis(p-chlorophe...	318	C14H10Cl4	000072-54-8	94
4			3-Butanone, 1,1-bis(4-chlorophen...	320	C18H18Cl2O	1000158-20-4	80
5			p,p'-DDT	352	C14H9Cl5	000050-29-3	72



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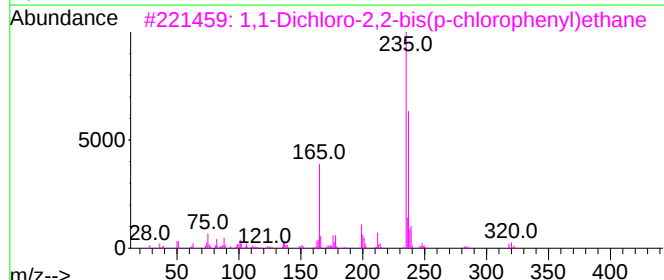
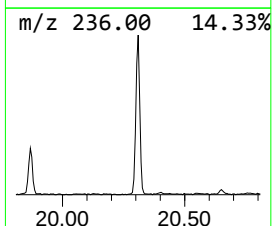
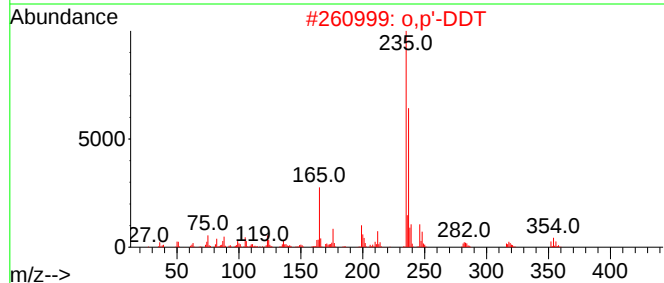
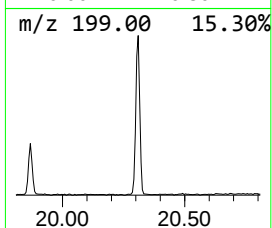
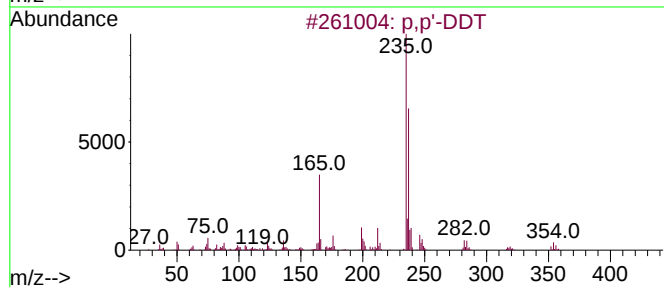
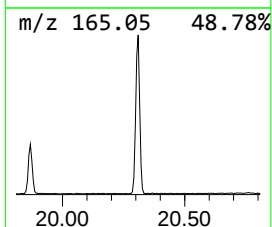
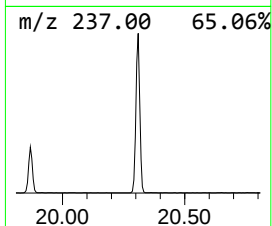
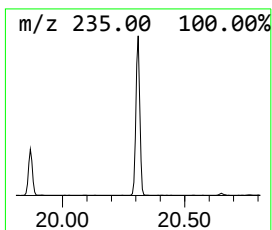
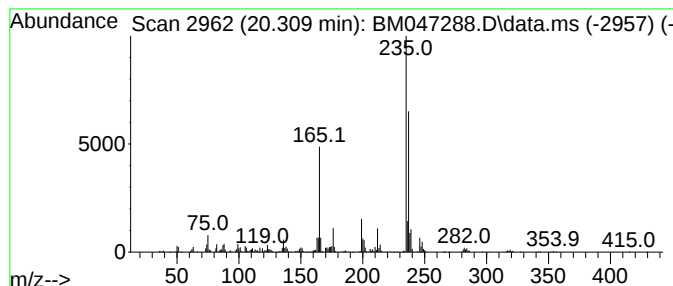
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Peak Number 4 p,p'-DDT Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.309	13.03 ng	1998830	Chrysene-d12	21.015

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			p,p'-DDT	352	C14H9Cl5	000050-29-3	98
2			o,p'-DDT	352	C14H9Cl5	000789-02-6	98
3			1,1-Dichloro-2,2-bis(p-chlorophe...	318	C14H10Cl4	000072-54-8	97
4			3-Butanone, 1,1-bis(4-chlorophen...	320	C18H18Cl2O	1000158-20-4	93
5			Mitotane	318	C14H10Cl4	000053-19-0	91



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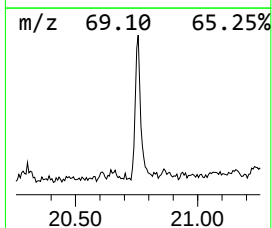
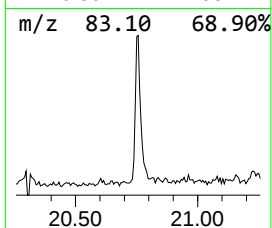
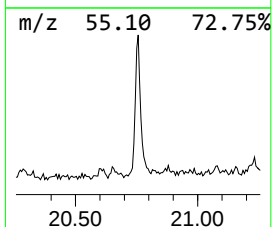
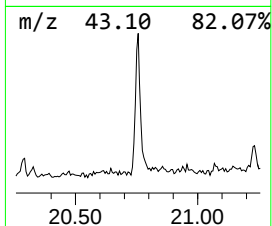
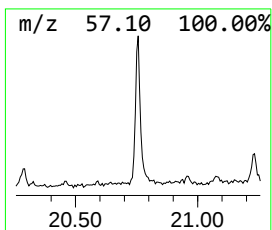
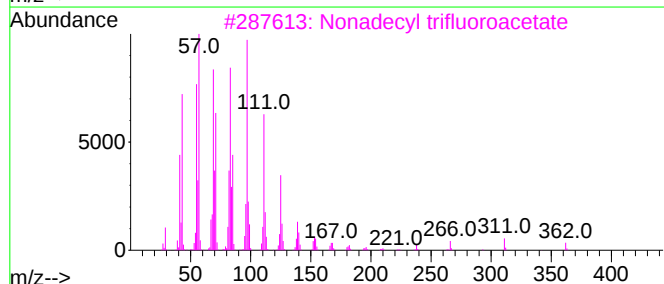
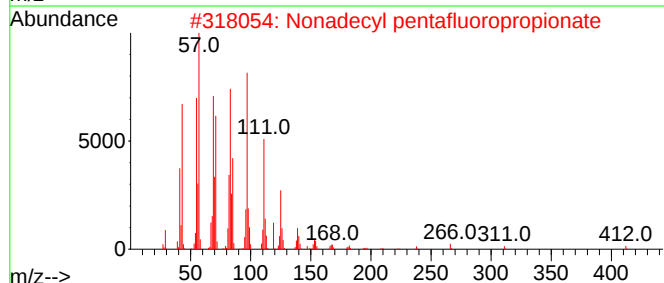
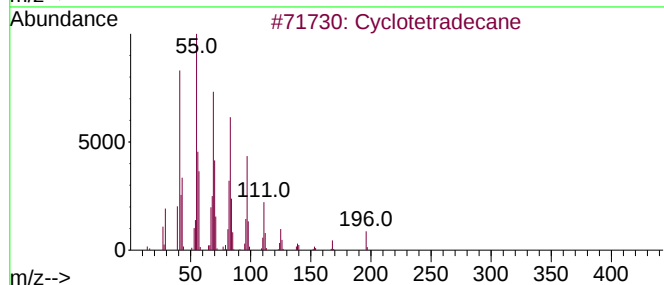
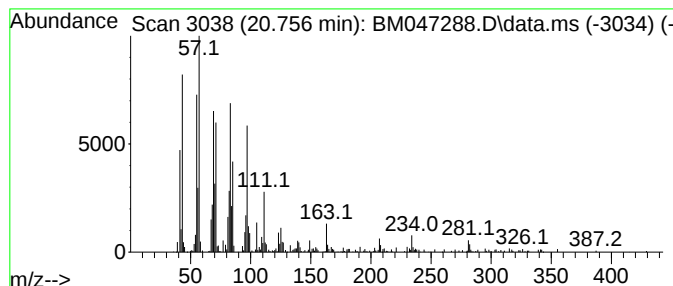
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Cyclotetradecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.756	2.03 ng	311286	Chrysene-d12	21.015

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclotetradecane	196	C14H28	000295-17-0	89
2			Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	83
3			Nonadecyl trifluoroacetate	380	C21H39F3O2	1000351-76-3	81
4			Pentadecafluorooctanoic acid, pe...	624	C23H31F15O2	1000406-04-5	81
5			1-Hexacosanol	382	C26H54O	000506-52-5	81



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM082024\
Data File : BM047288.D
Acq On : 21 Aug 2024 02:52
Operator : RC/JU
Sample : P3580-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
926-K1-SD-0-0.5-081224

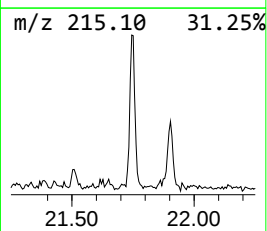
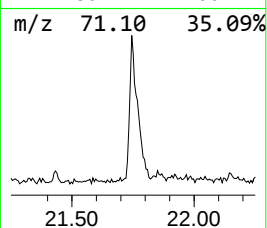
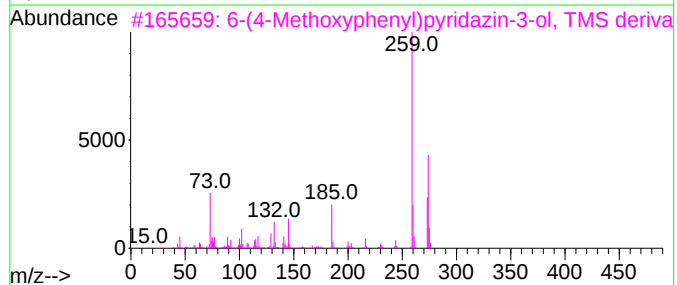
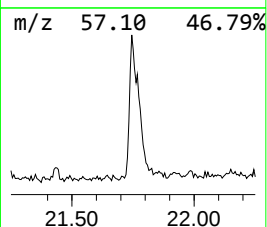
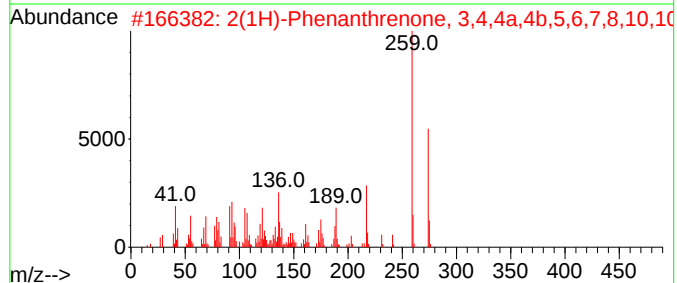
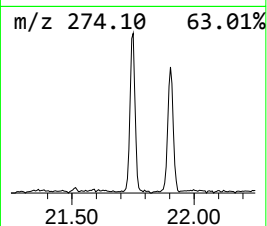
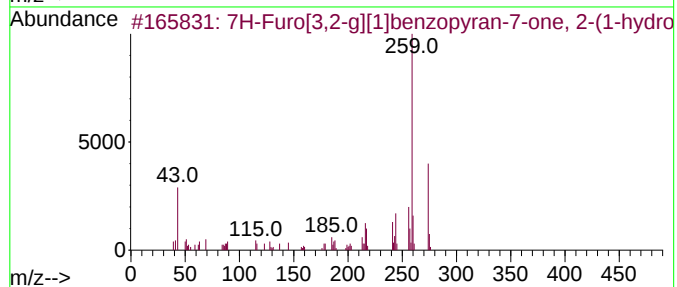
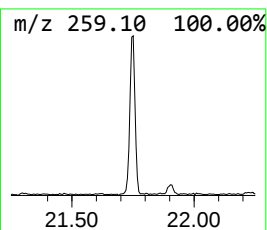
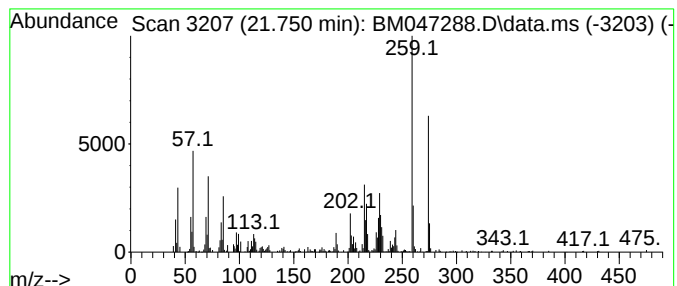
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 7H-Furo[3,2-g][1]benzopyran... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.750	4.20 ng	645012	Chrysene-d12	21.015

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			7H-Furo[3,2-g][1]benzopyran-7-on...	274	C15H14O5	054087-32-0	58
2			2(1H)-Phenanthrenone, 3,4,4a,4b,...	274	C19H30O	007715-44-8	52
3			6-(4-Methoxyphenyl)pyridazin-3-o...	274	C14H18N2O2Si	1000476-89-3	50
4			Xanthotoxol, trimethylsilyl ether	274	C14H14O4Si	1000462-10-7	49
5			9-Methyl-3-phenyl-9H-pyridazino(...	259	C17H13N3	003980-90-3	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM082024\
Data File : BM047288.D
Acq On : 21 Aug 2024 02:52
Operator : RC/JU
Sample : P3580-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
926-K1-SD-0-0.5-081224

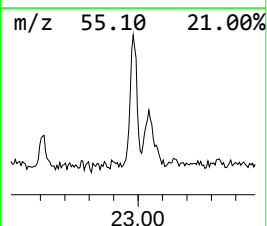
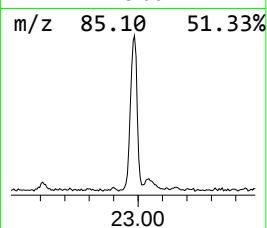
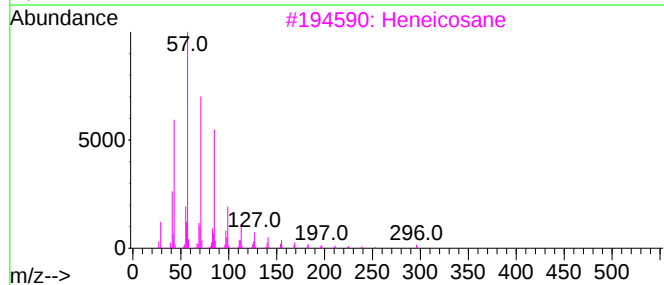
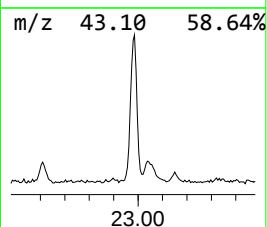
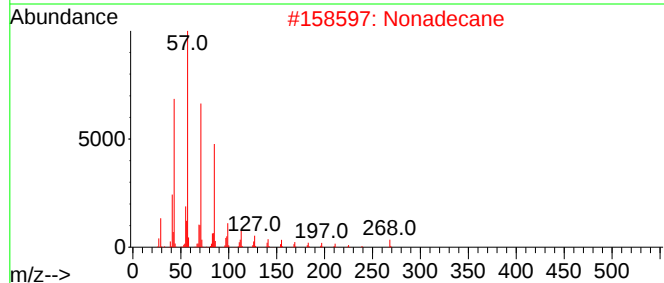
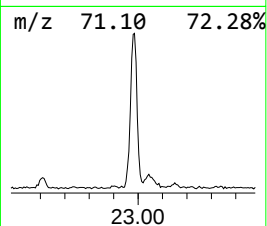
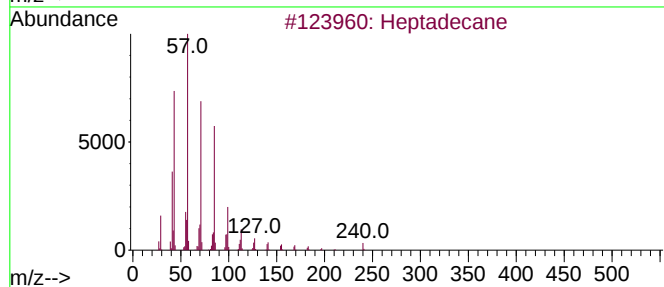
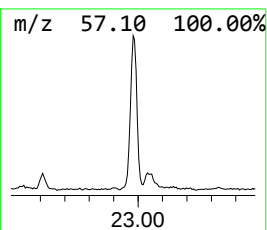
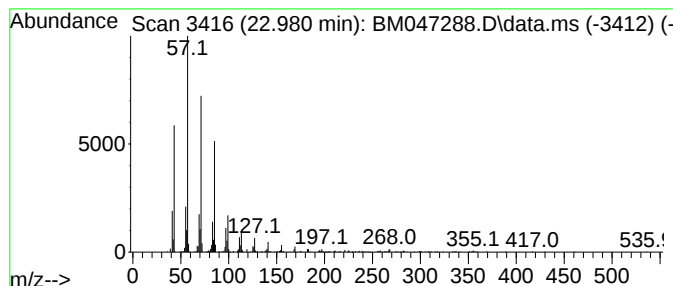
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Heptadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.980	3.73 ng	562635	Perylene-d12	23.715

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptadecane	240	C17H36	000629-78-7	95
2			Nonadecane	268	C19H40	000629-92-5	93
3			Heneicosane	296	C21H44	000629-94-7	91
4			Triacontane, 1-iodo-	548	C30H61I	1000406-32-3	91
5			Hexatriacontane	507	C36H74	000630-06-8	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM082024\
Data File : BM047288.D
Acq On : 21 Aug 2024 02:52
Operator : RC/JU
Sample : P3580-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
926-K1-SD-0-0.5-081224

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM081024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	4.569	2.9	ng	263327	1	7.357	1819890	20.0
n-Hexadecanoic ...	17.715	2.5	ng	349654	4	16.780	2829140	20.0
Mitotane	19.868	3.9	ng	599907	5	21.015	3068960	20.0
p,p'-DDT	20.309	13.0	ng	1998830	5	21.015	3068960	20.0
Cyclotetradecane	20.756	2.0	ng	311286	5	21.015	3068960	20.0
7H-Furo[3,2-g][...	21.750	4.2	ng	645012	5	21.015	3068960	20.0
Heptadecane	22.980	3.7	ng	562635	6	23.715	3017710	20.0