

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM031521\
 Data File : BM029139.D
 Acq On : 15 Mar 2021 20:38
 Operator : CG/JU
 Sample : M1664-02
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 VNJ-230

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-BM022321.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM029139.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.193	370	375	389	rBB	111473	162918	45.55%	6.357%
2	6.810	645	650	667	rBB	106209	174220	48.71%	6.798%
3	7.616	781	787	793	rBB	28225	42600	11.91%	1.662%
4	8.786	980	986	997	rBB	68869	109814	30.70%	4.285%
5	10.398	1255	1260	1269	rBB	36902	59001	16.50%	2.302%
6	12.892	1679	1684	1692	rBB	160876	222600	62.24%	8.685%
7	14.286	1915	1921	1926	rBB	51771	73027	20.42%	2.849%
8	15.786	2171	2176	2183	rBB	135209	173778	48.59%	6.781%
9	16.704	2328	2332	2336	rBB	4224	4786	1.34%	0.187%
10	17.033	2383	2388	2392	rBV	63271	84605	23.66%	3.301%
11	17.074	2392	2395	2401	rVB	17067	21994	6.15%	0.858%
12	17.933	2531	2541	2552	rBV	59101	85326	23.86%	3.329%
13	18.098	2561	2569	2573	rVB4	3123	5432	1.52%	0.212%
14	18.468	2628	2632	2636	rBV2	4118	5196	1.45%	0.203%
15	18.509	2636	2639	2643	rVB2	4223	4824	1.35%	0.188%
16	18.668	2662	2666	2671	rVB	7064	9087	2.54%	0.355%
17	19.092	2732	2738	2750	rBV2	62926	88782	24.82%	3.464%
18	19.215	2755	2759	2768	rBV	45920	62198	17.39%	2.427%
19	19.427	2791	2795	2796	rBV	6058	6599	1.85%	0.257%
20	19.456	2796	2800	2806	rVB	42764	56766	15.87%	2.215%
21	19.662	2828	2835	2840	rBV	296926	357647	100.00%	13.955%
22	19.786	2851	2856	2861	rVB3	1827	4127	1.15%	0.161%
23	19.956	2880	2885	2889	rVB5	4739	7813	2.18%	0.305%
24	20.056	2899	2902	2906	rVB2	3375	3653	1.02%	0.143%
25	20.115	2906	2912	2915	rBV3	4154	6527	1.82%	0.255%
26	20.297	2939	2943	2949	rVB4	4635	6767	1.89%	0.264%
27	20.709	3010	3013	3019	rVB2	4775	5819	1.63%	0.227%
28	20.868	3035	3040	3043	rVV	8289	11076	3.10%	0.432%
29	20.927	3043	3050	3060	rVV5	40093	65112	18.21%	2.541%
30	21.003	3060	3063	3067	rVB	5533	6756	1.89%	0.264%
31	21.127	3080	3084	3089	rVB	54356	56112	15.69%	2.189%
32	21.215	3092	3099	3103	rVV2	111396	172011	48.10%	6.712%
33	21.250	3103	3105	3113	rVB	31121	34634	9.68%	1.351%
34	21.368	3121	3125	3128	rBV4	7473	10385	2.90%	0.405%
35	21.797	3196	3198	3206	rVB6	12484	18467	5.16%	0.721%
36	22.686	3346	3349	3351	rBV	17994	22472	6.28%	0.877%

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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-BM022321.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	22.721	3352	3355	3366	rVB2	32571	96484	26.98%	3.765%
38	23.168	3428	3431	3436	rVB	15352	21429	5.99%	0.836%
39	23.262	3443	3447	3454	rVB	23266	39041	10.92%	1.523%
40	23.350	3456	3462	3468	rBV2	70461	121599	34.00%	4.745%
41	23.815	3536	3541	3547	rVB	24577	41423	11.58%	1.616%

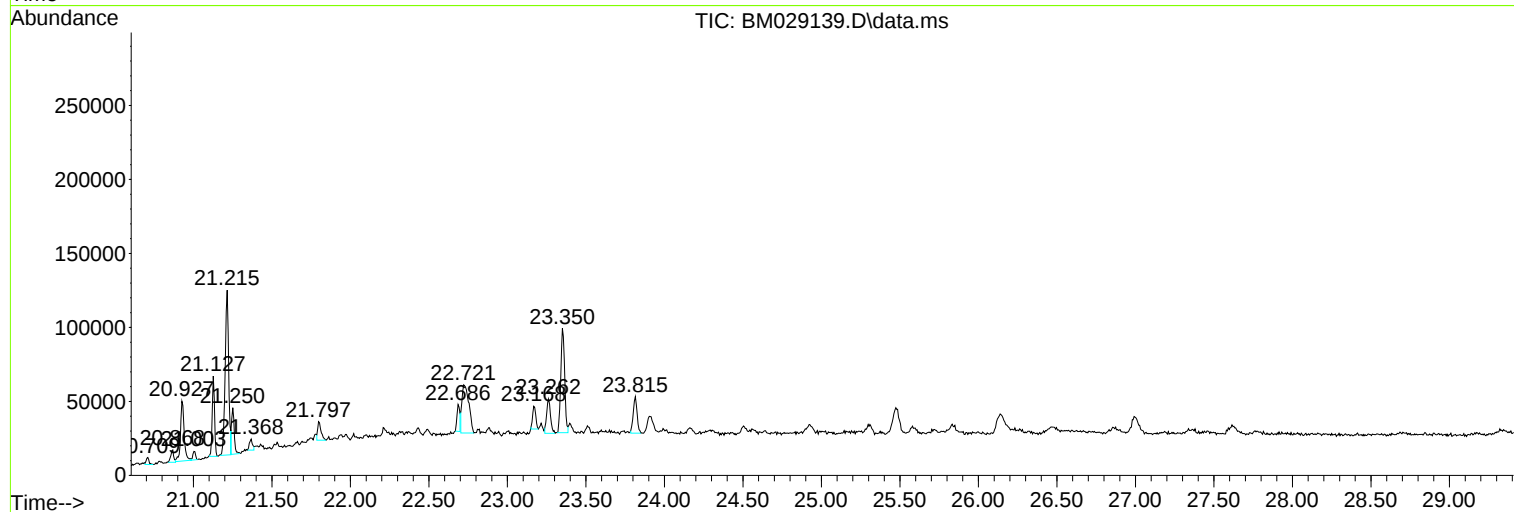
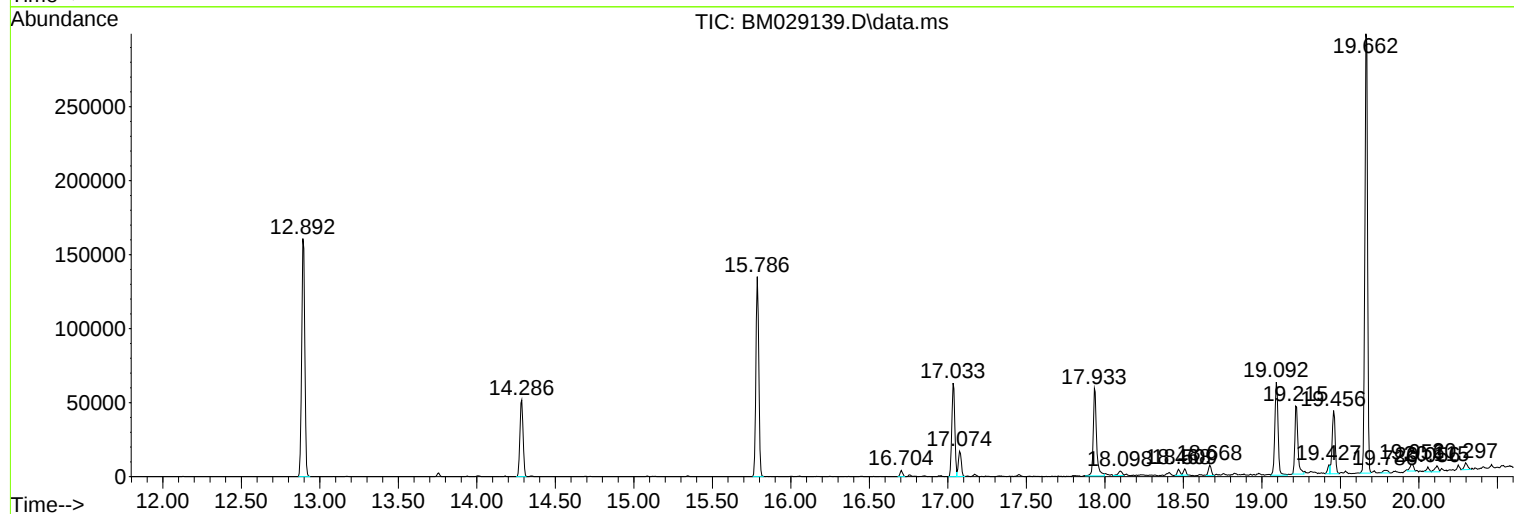
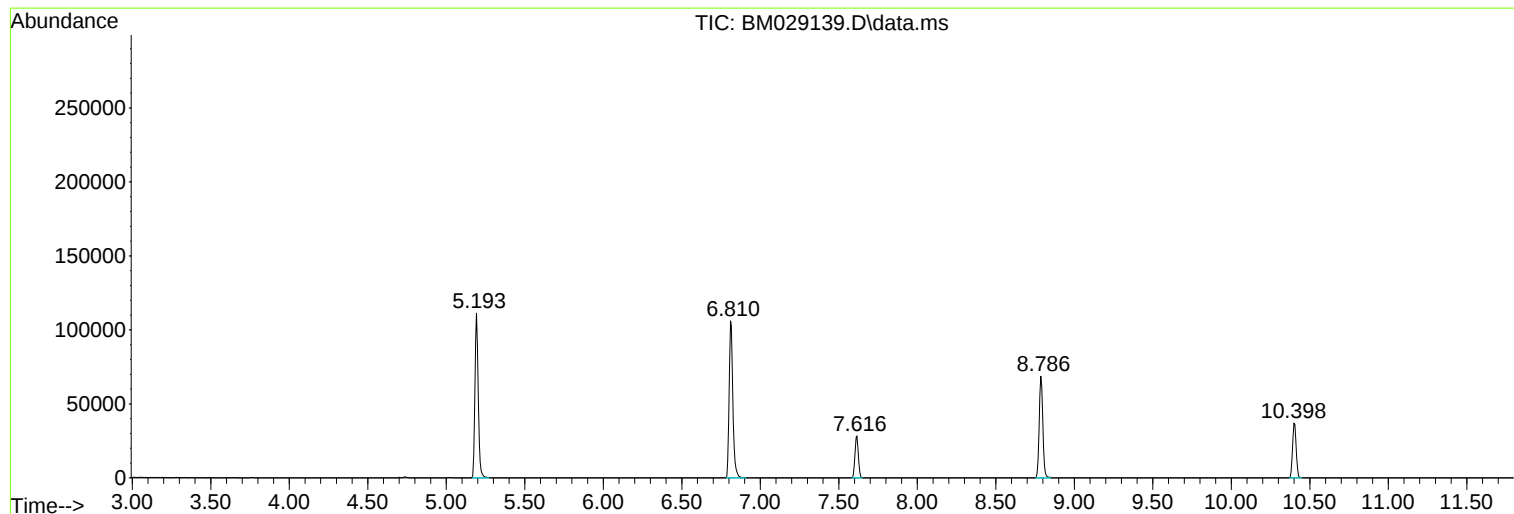
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM022321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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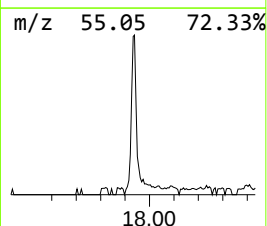
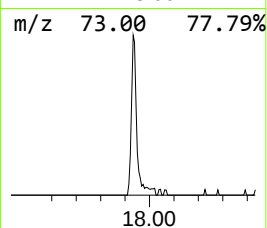
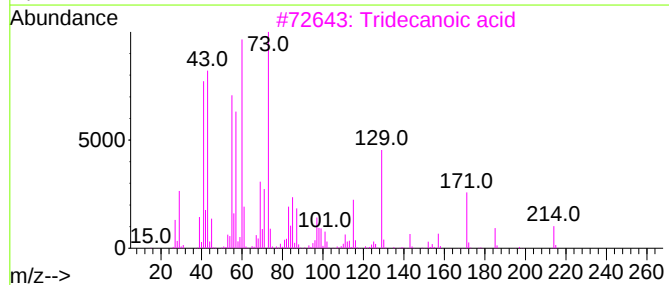
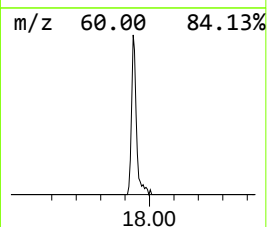
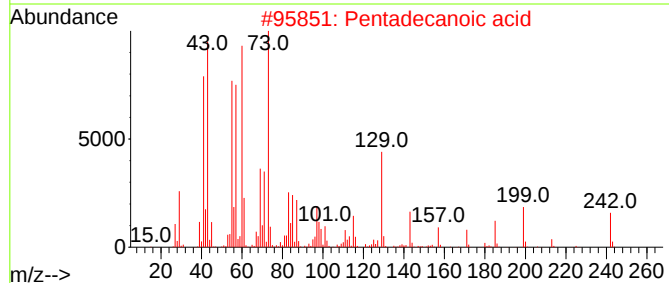
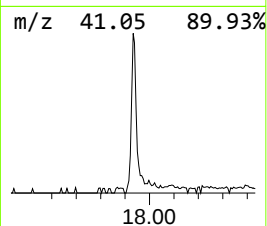
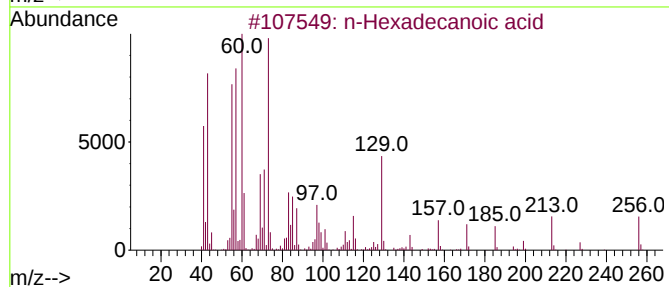
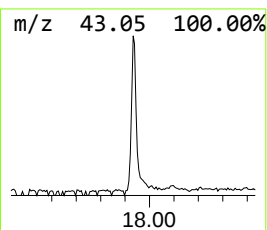
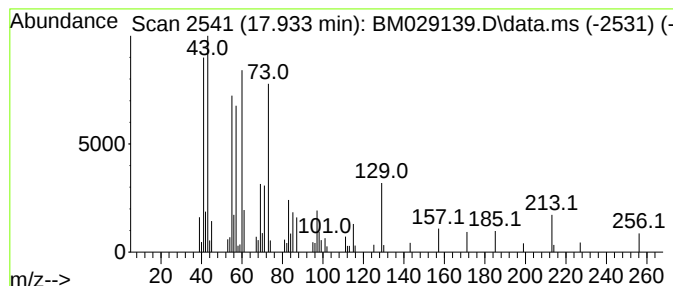
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM022321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.933	20.17 ng	85326	Phenanthrene-d10	17.033

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3			Tridecanoic acid	214	C13H26O2	000638-53-9	76
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5			11-Bromoundecanoic acid	264	C11H21BrO2	002834-05-1	53



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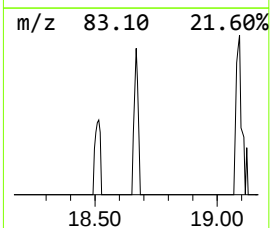
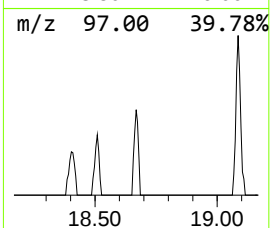
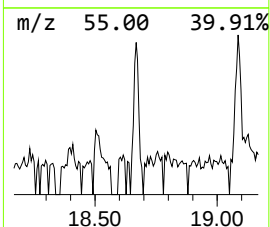
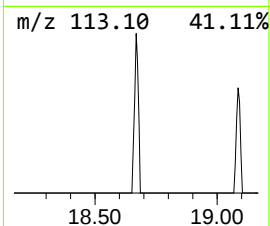
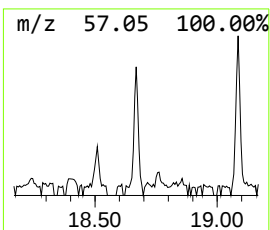
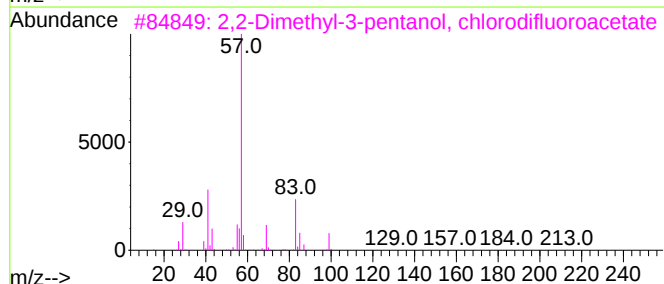
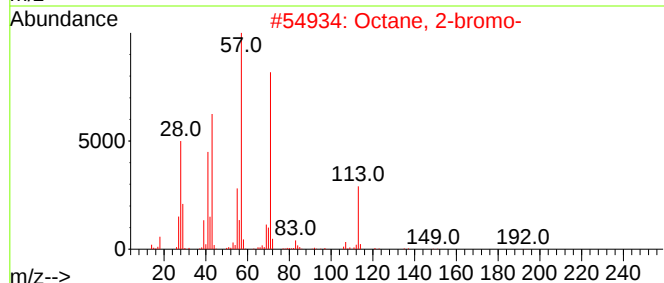
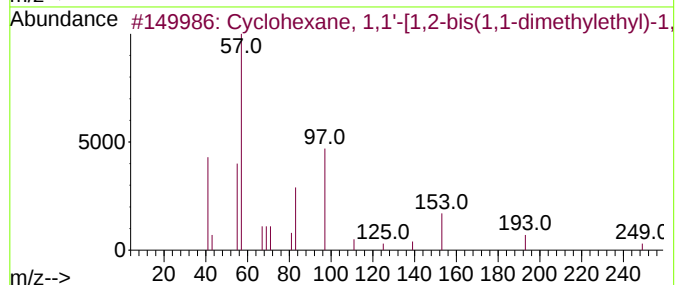
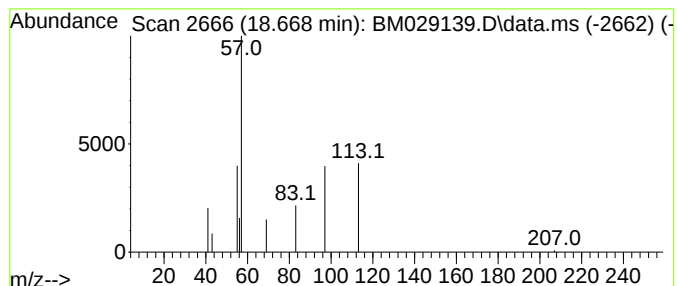
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown18.668 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.668	2.15 ng	9087	Phenanthrene-d10	17.033

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexane, 1,1'-[1,2-bis(1,1-d...	306	C22H42	065149-85-1	40
2			Octane, 2-bromo-	192	C8H17Br	000557-35-7	25
3			2,2-Dimethyl-3-pentanol, chlorod...	228	C9H15ClF2O2	1000376-26-4	12
4			Pentane, 2,2,4-trimethyl-4-nitro-	159	C8H17NO2	005342-78-9	9
5			2,2-Dimethyl-3-pentanol, heptafl...	312	C11H15F7O2	1000364-14-4	9



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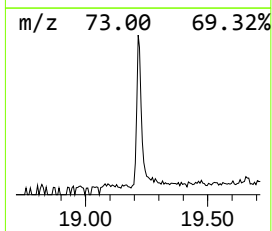
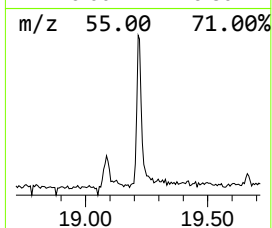
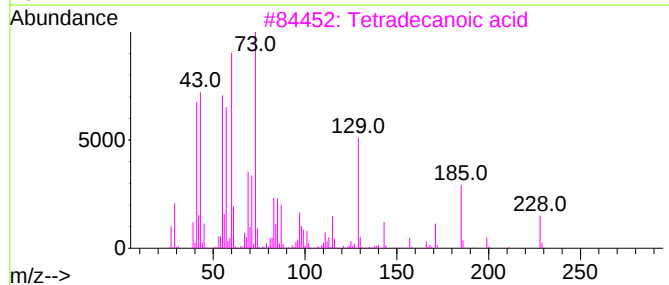
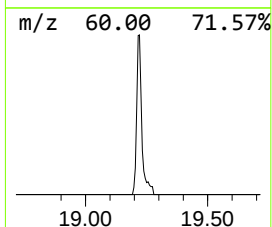
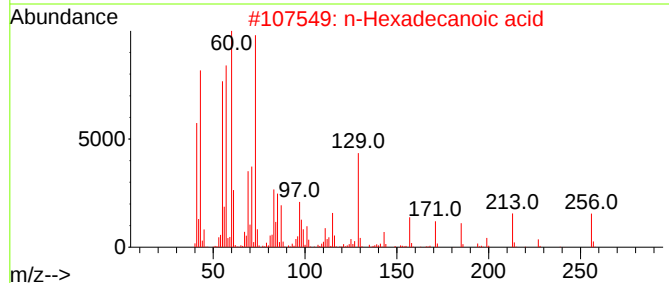
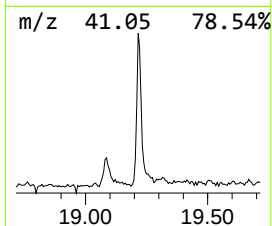
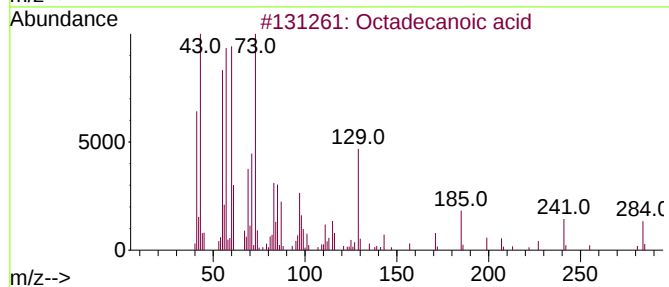
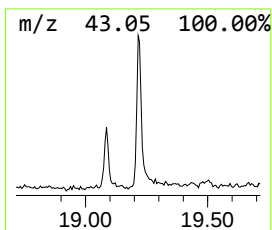
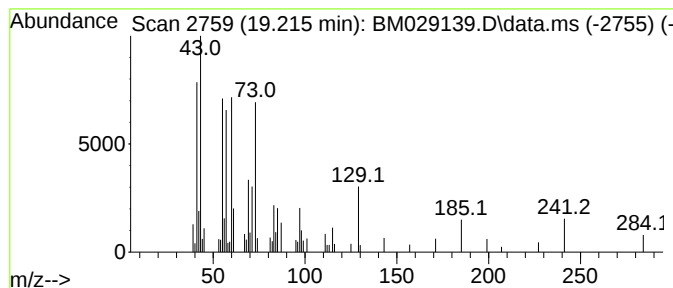
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Octadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.215	7.23 ng	62198	Chrysene-d12	21.215

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	87
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	83
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	80
5			n-Decanoic acid	172	C10H20O2	000334-48-5	35



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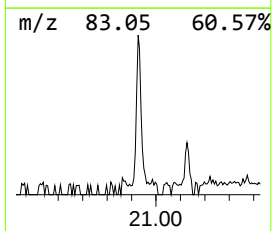
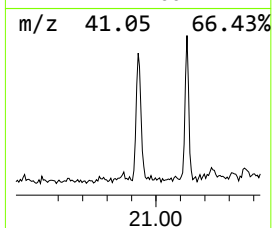
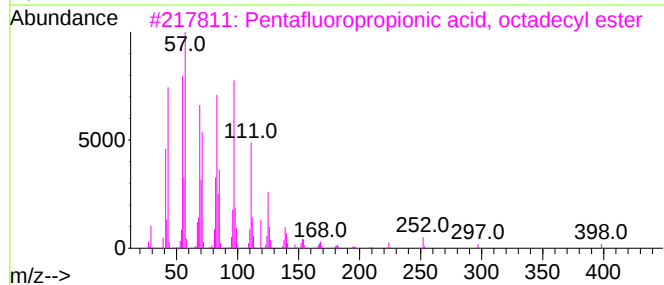
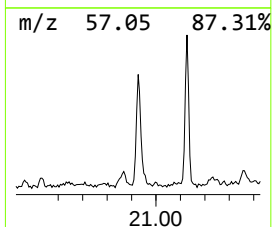
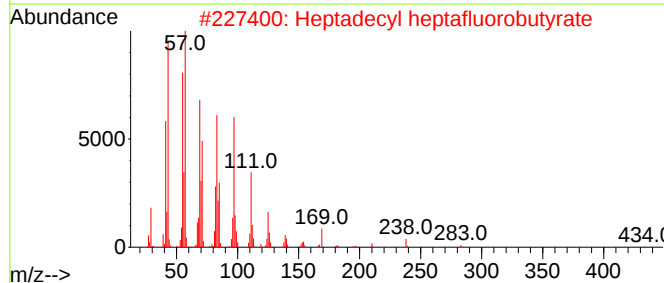
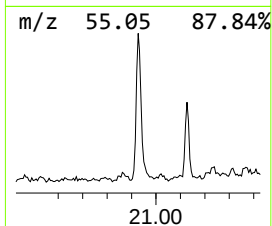
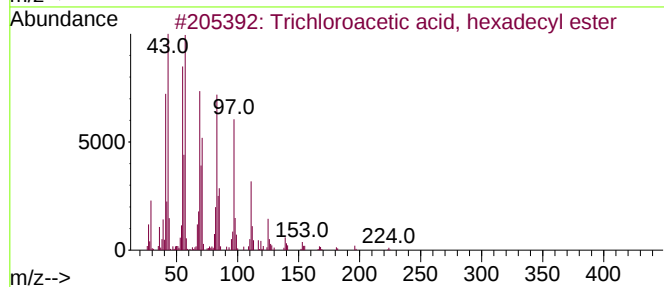
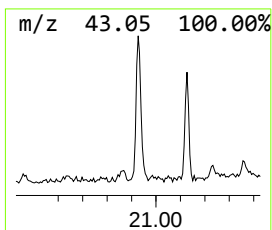
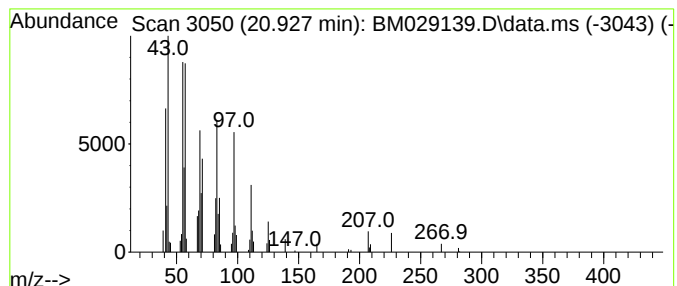
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 4 Trichloroacetic acid, hexad... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.927	7.57 ng	65112	Chrysene-d12	21.215

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	95
2			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
3			Pentafluoropropionic acid, octad...	416	C21H37F5O2	959261-25-7	91
4			Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	91
5			Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	91



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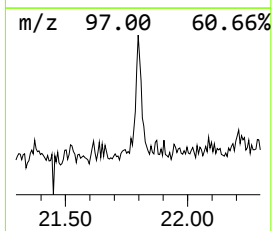
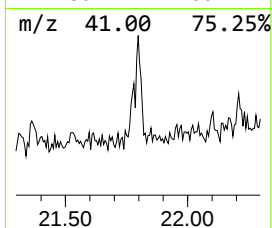
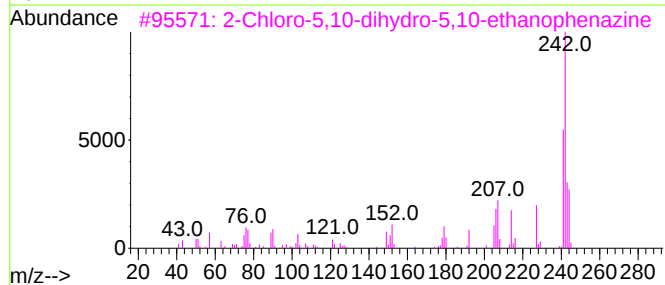
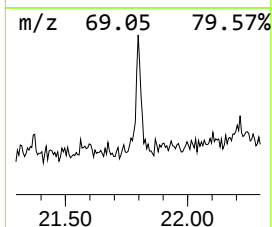
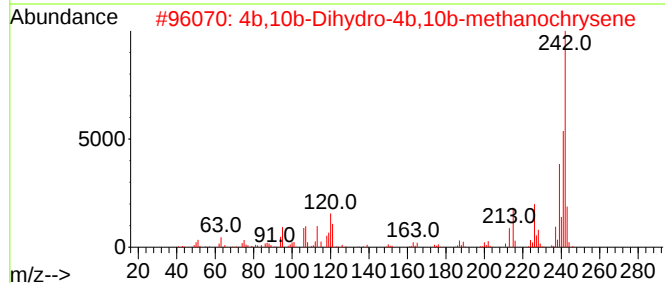
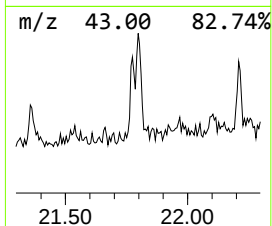
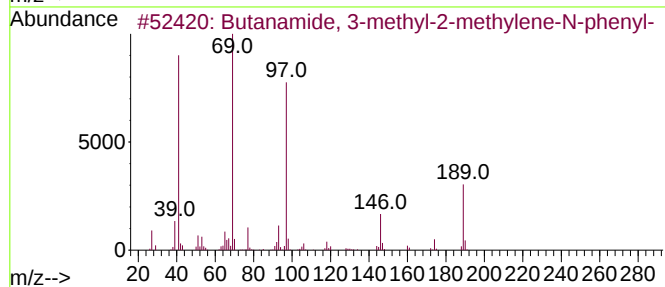
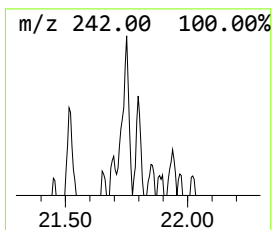
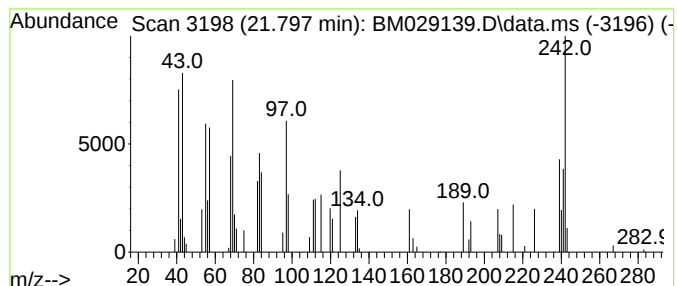
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 unknown21.797 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.797	2.15 ng	18467	Chrysene-d12	21.215

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanamide, 3-methyl-2-methylene...	189	C12H15NO	095383-63-4	25
2			4b,10b-Dihydro-4b,10b-methanochr...	242	C19H14	071949-03-6	25
3			2-Chloro-5,10-dihydro-5,10-ethan...	242	C14H11ClN2	1000110-61-2	22
4			Chrysene, 1-methyl-	242	C19H14	003351-28-8	16
5			2-Methylchrysene	242	C19H14	003351-32-4	16



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM031521\
Data File : BM029139.D
Acq On : 15 Mar 2021 20:38
Operator : CG/JU
Sample : M1664-02
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
VNJ-230

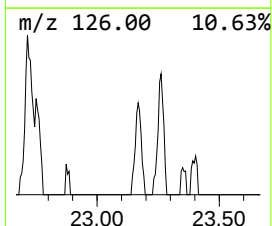
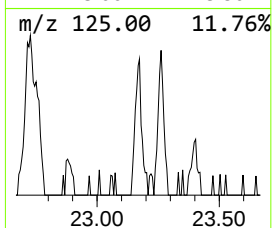
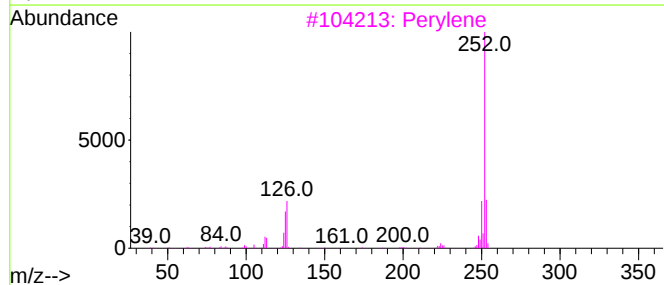
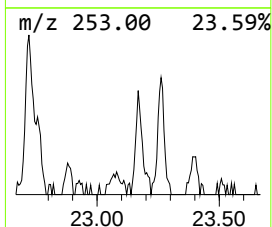
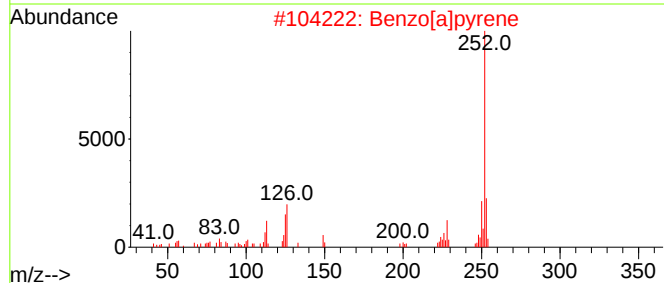
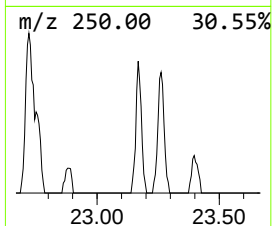
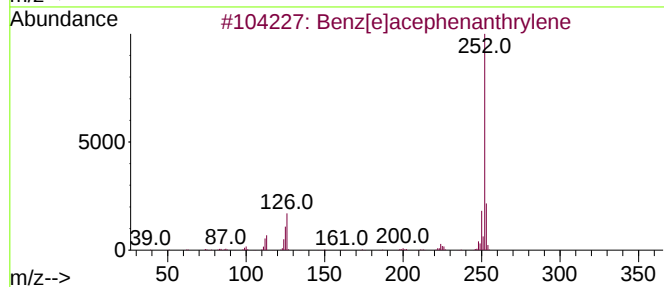
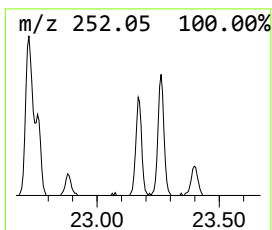
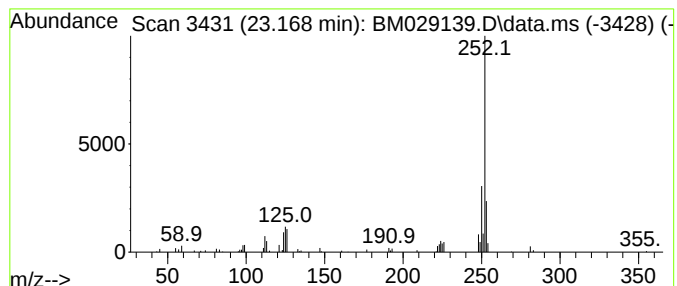
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Perylene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.168	3.52 ng	21429	Perylene-d12	23.350

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benz[e]acephenanthrylene	252	C20H12	000205-99-2	90
2			Benzo[a]pyrene	252	C20H12	000050-32-8	89
3			Perylene	252	C20H12	000198-55-0	81
4			Benzo[k]fluoranthene	252	C20H12	000207-08-9	81
5			Benzo[e]pyrene	252	C20H12	000192-97-2	81



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM031521\
Data File : BM029139.D
Acq On : 15 Mar 2021 20:38
Operator : CG/JU
Sample : M1664-02
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
VNJ-230

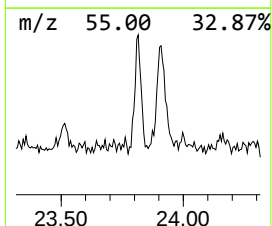
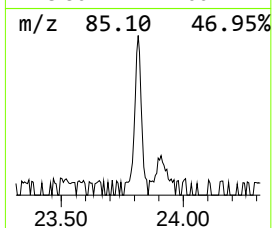
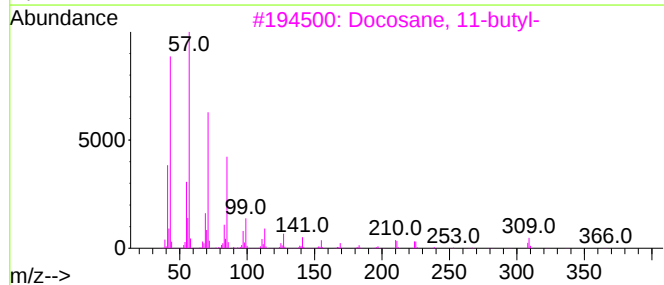
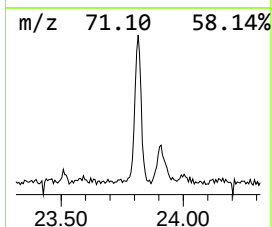
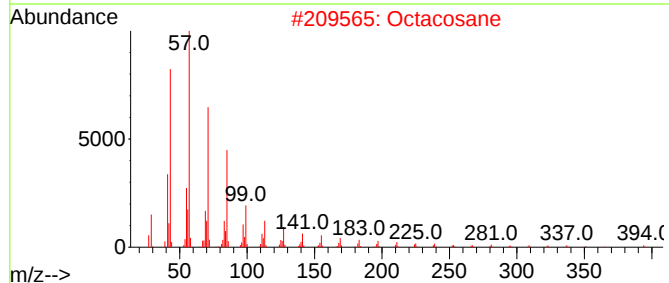
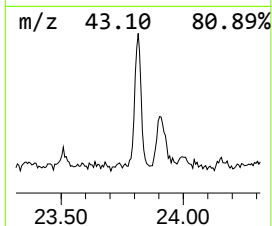
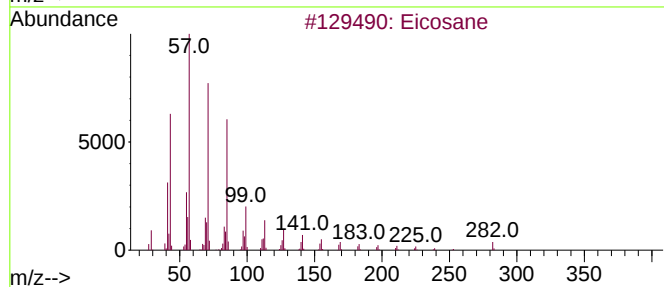
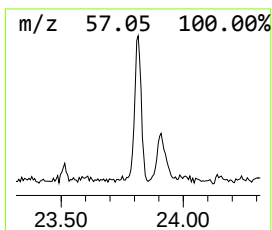
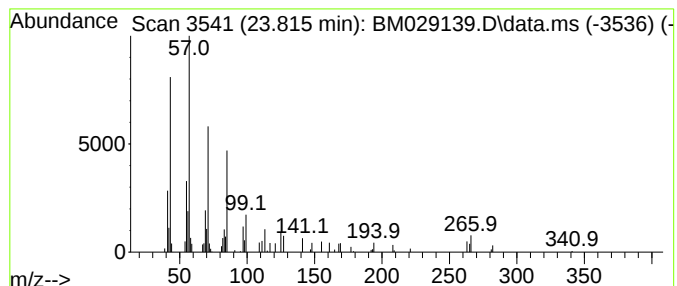
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Eicosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.815	6.81 ng	41423	Perylene-d12	23.350

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eicosane	282	C20H42	000112-95-8	96
2			Octacosane	394	C28H58	000630-02-4	76
3			Docosane, 11-butyl-	366	C26H54	013475-76-8	76
4			Tetracosane	338	C24H50	000646-31-1	76
5			Heptacosane	380	C27H56	000593-49-7	76



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM031521\
Data File : BM029139.D
Acq On : 15 Mar 2021 20:38
Operator : CG/JU
Sample : M1664-02
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
VNJ-230

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM022321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
n-Hexadecanoic ...	17.933	20.2	ng	85326	4	17.033	84605	20.0
unknown18.668	18.668	2.1	ng	9087	4	17.033	84605	20.0
Octadecanoic acid	19.215	7.2	ng	62198	5	21.215	172011	20.0
Trichloroacetic...	20.927	7.6	ng	65112	5	21.215	172011	20.0
unknown21.797	21.797	2.1	ng	18467	5	21.215	172011	20.0
Perylene	23.168	3.5	ng	21429	6	23.350	121599	20.0
Eicosane	23.815	6.8	ng	41423	6	23.350	121599	20.0