

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG082923\
 Data File : BG058887.D
 Acq On : 29 Aug 2023 14:42
 Operator : MA/JU
 Sample : 04165-03
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 VNJ-210

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_G\Methods\8270-BG081823.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG058887.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.358	380	386	398	rBV	319846	499702	38.55%	6.220%
2	6.962	652	659	671	rBV	336149	565436	43.62%	7.039%
3	7.785	792	799	807	rVB	62538	100904	7.78%	1.256%
4	8.948	990	997	1009	rBV	195132	343968	26.53%	4.282%
5	10.587	1269	1276	1284	rBV	90428	163207	12.59%	2.032%
6	13.055	1689	1696	1706	rBV	569408	868649	67.01%	10.813%
7	13.325	1736	1742	1749	rVB	45703	68770	5.30%	0.856%
8	14.436	1925	1931	1938	rBV	168974	254841	19.66%	3.172%
9	15.928	2177	2185	2195	rBV	523609	804614	62.07%	10.016%
10	17.186	2393	2399	2403	rBV	201253	318482	24.57%	3.965%
11	17.227	2403	2406	2411	rVB	43197	58530	4.52%	0.729%
12	18.073	2543	2550	2554	rBV2	99400	154004	11.88%	1.917%
13	18.249	2575	2580	2584	rBV4	12221	22989	1.77%	0.286%
14	18.607	2637	2641	2646	rBV6	10928	16235	1.25%	0.202%
15	19.124	2723	2729	2735	rBV6	8817	20360	1.57%	0.253%
16	19.242	2740	2749	2757	rVV	128132	192394	14.84%	2.395%
17	19.348	2762	2767	2778	rBV5	37237	60754	4.69%	0.756%
18	19.571	2801	2805	2807	rBV2	26518	36514	2.82%	0.455%
19	19.606	2807	2811	2818	rVB	109920	162116	12.51%	2.018%
20	19.677	2818	2823	2827	rBV7	11066	19492	1.50%	0.243%
21	19.806	2838	2845	2850	rBV	1003409	1296328	100.00%	16.137%
22	19.929	2860	2866	2873	rBV5	12822	32352	2.50%	0.403%
23	20.070	2885	2890	2892	rBV5	13488	23836	1.84%	0.297%
24	20.100	2892	2895	2899	rVB2	30636	40491	3.12%	0.504%
25	20.258	2915	2922	2925	rBV3	18318	33752	2.60%	0.420%
26	20.441	2950	2953	2957	rVV3	10871	15013	1.16%	0.187%
27	20.599	2976	2980	2984	rVB3	18187	21867	1.69%	0.272%
28	20.852	3019	3023	3028	rVB	17449	29096	2.24%	0.362%
29	21.022	3050	3052	3056	rBV4	10339	14708	1.13%	0.183%
30	21.075	3057	3061	3073	rVB5	78561	146721	11.32%	1.826%
31	21.163	3073	3076	3081	rVB3	14715	23716	1.83%	0.295%
32	21.304	3098	3100	3106	rVB	17871	22834	1.76%	0.284%
33	21.422	3112	3120	3125	rBV3	228088	443741	34.23%	5.524%
34	21.463	3125	3127	3135	rVB	60741	84342	6.51%	1.050%
35	22.115	3234	3238	3243	rVB	13868	22253	1.72%	0.277%
36	22.186	3243	3250	3260	rBV7	36008	93759	7.23%	1.167%

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Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	22.515	3304	3306	3311	rVB5	13588	17158	1.32%	0.214%
38	22.991	3382	3387	3397	rVB	50750	100080	7.72%	1.246%
39	23.508	3469	3475	3481	rBV2	47174	126874	9.79%	1.579%
40	23.566	3482	3485	3491	rVB3	42264	72339	5.58%	0.900%
41	24.183	3585	3590	3591	rBV5	27844	36493	2.82%	0.454%
42	24.330	3609	3615	3626	rVB	44776	123082	9.49%	1.532%
43	24.477	3630	3640	3648	rBV	133855	367445	28.35%	4.574%
44	27.949	4220	4231	4248	rVB3	22965	113055	8.72%	1.407%

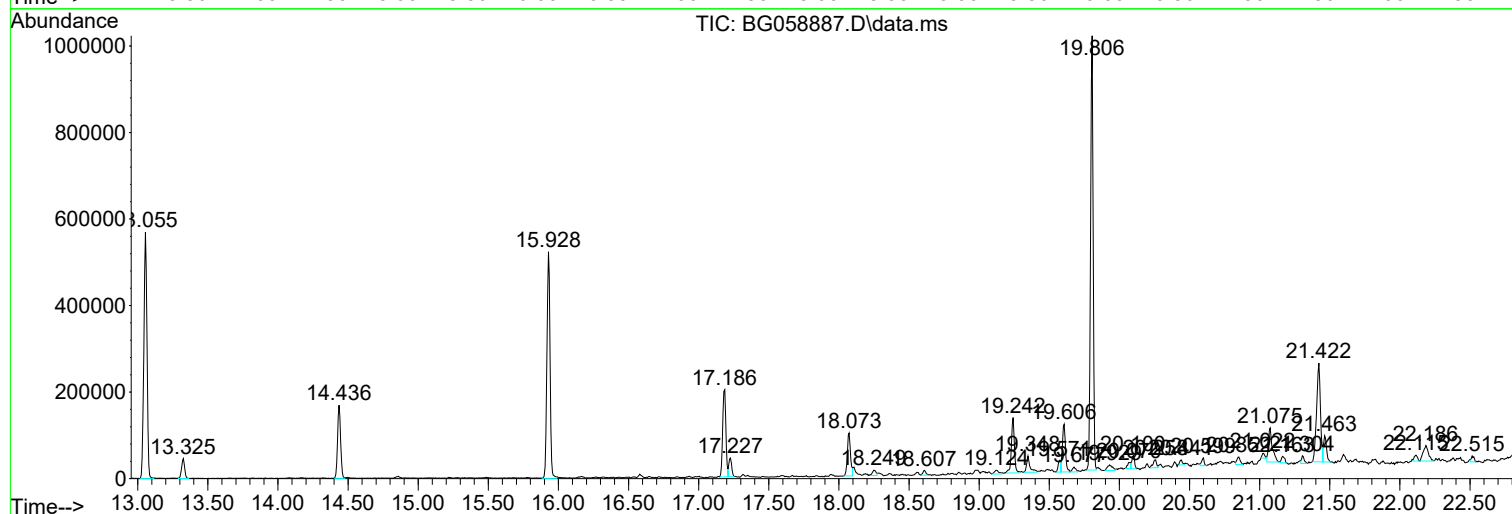
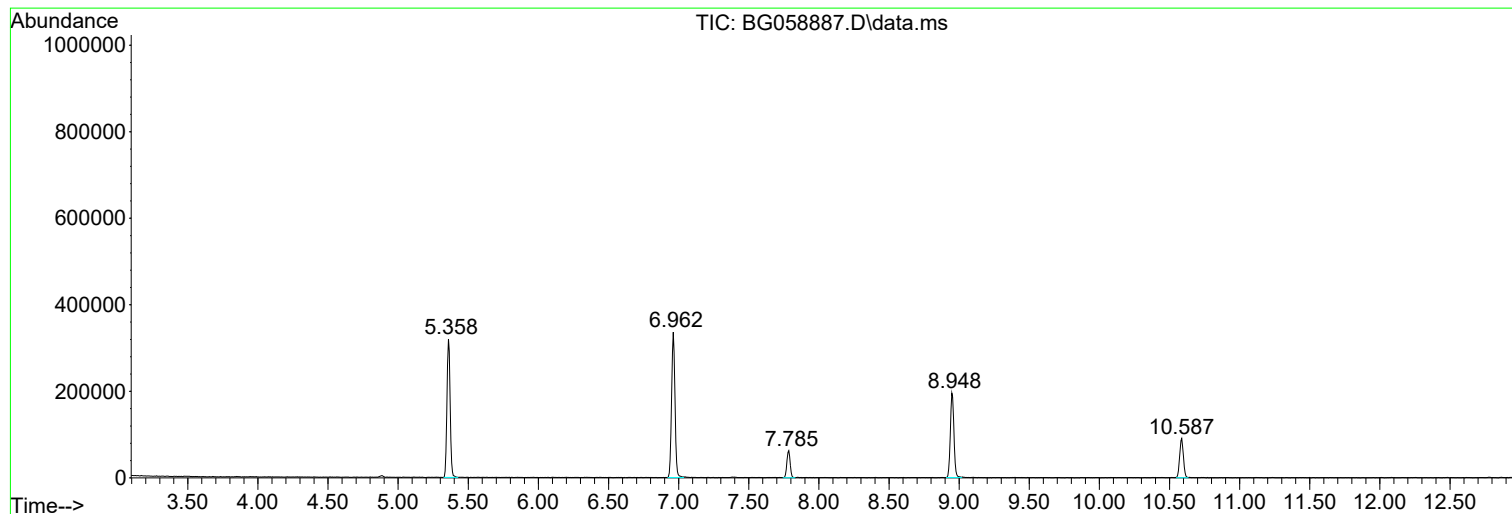
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG081823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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ALS Vial : 6 Sample Multiplier: 1

Instrument :
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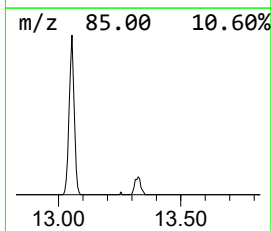
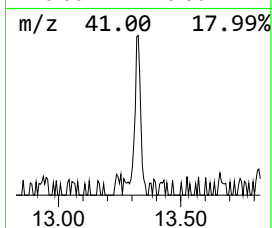
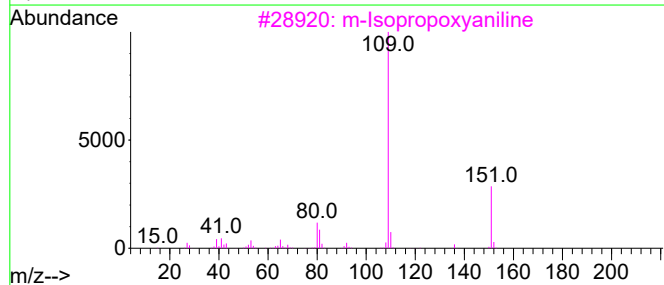
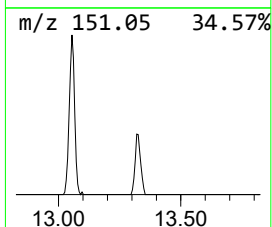
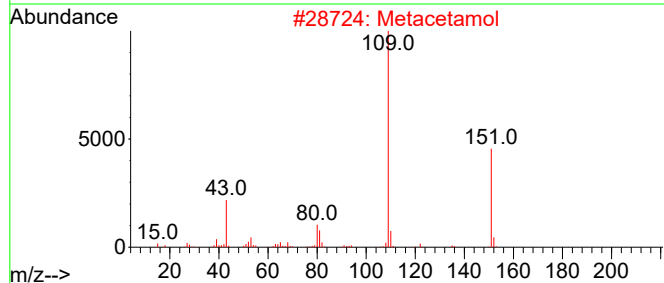
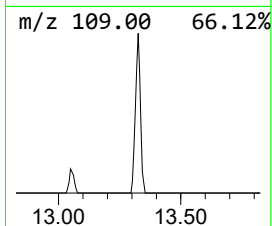
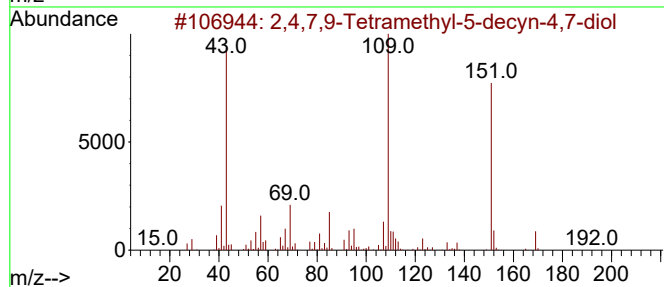
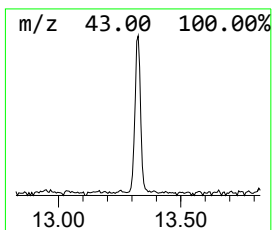
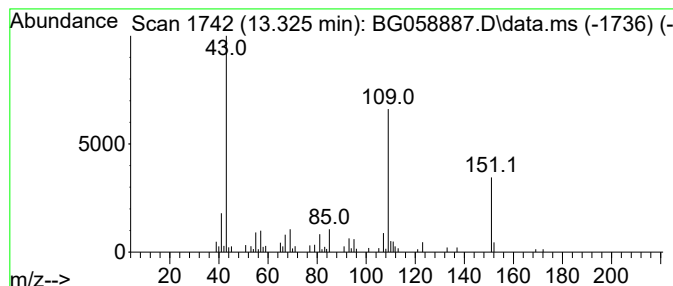
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.325	5.40 ng	68770	Acenaphthene-d10	14.436

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2		000126-86-3	91
2	Metacetamol	151	C8H9NO2		000621-42-1	52
3	m-Isopropoxyaniline	151	C9H13NO		041406-00-2	50
4	Acetaminophen	151	C8H9NO2		000103-90-2	50
5	Pyridine, 2-butyl-, 1-oxide	151	C9H13NO		031396-32-4	50



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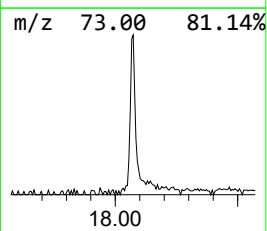
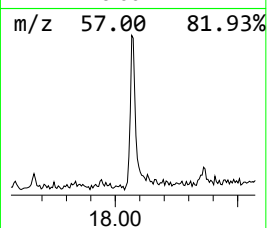
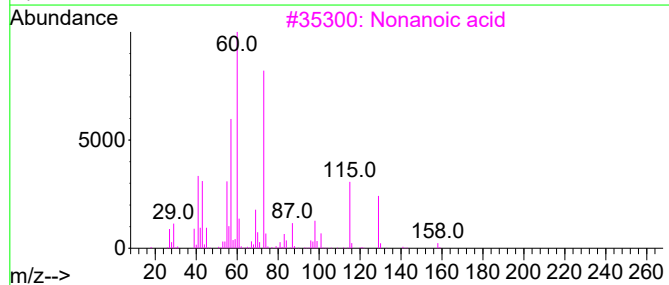
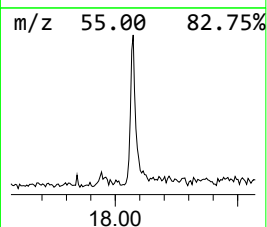
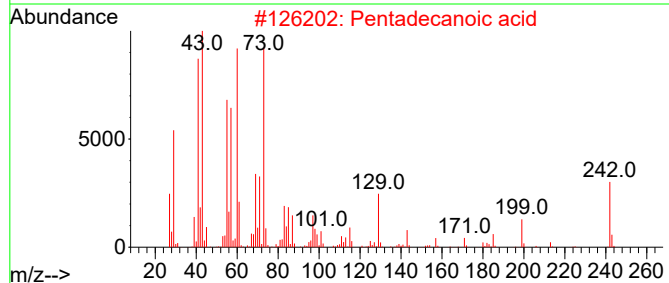
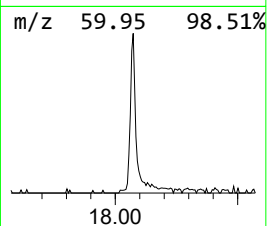
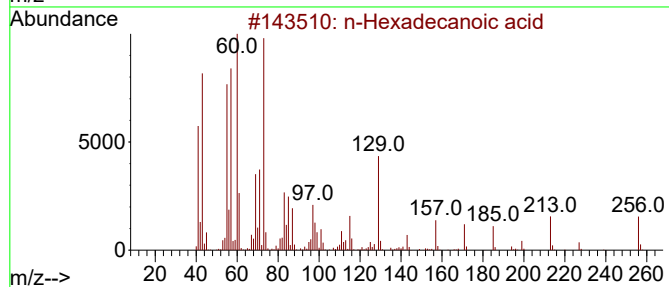
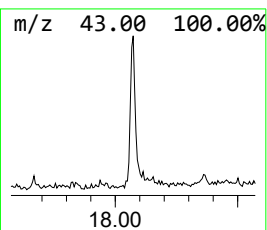
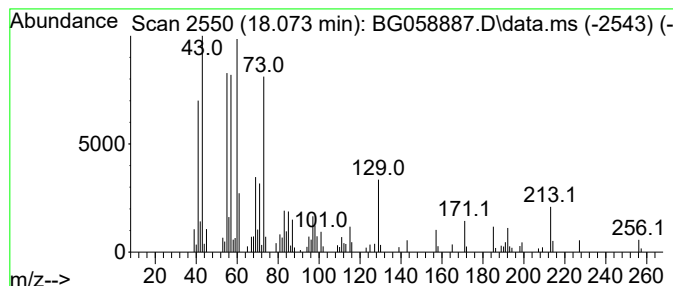
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.073	9.67 ng	154004	Phenanthrene-d10	17.186

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	90
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	64
3		Nonanoic acid	158	C9H18O2	000112-05-0	60
4		Tridecanoic acid	214	C13H26O2	000638-53-9	58
5		Tetradecanoic acid	228	C14H28O2	000544-63-8	53



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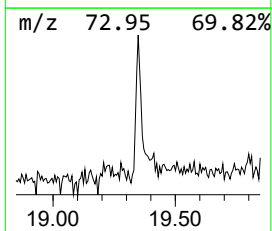
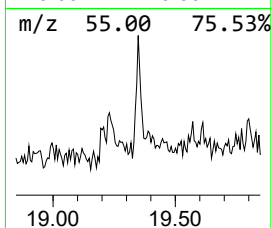
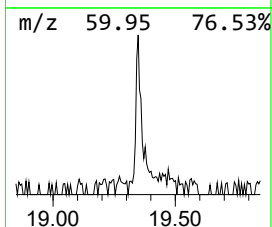
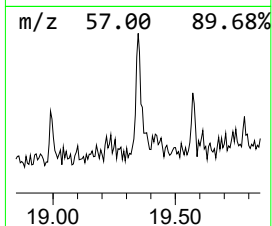
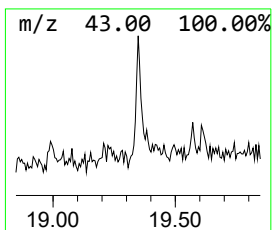
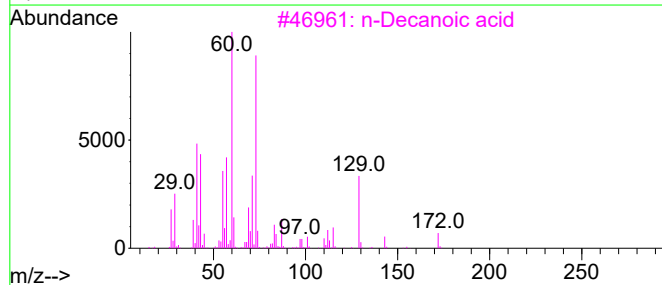
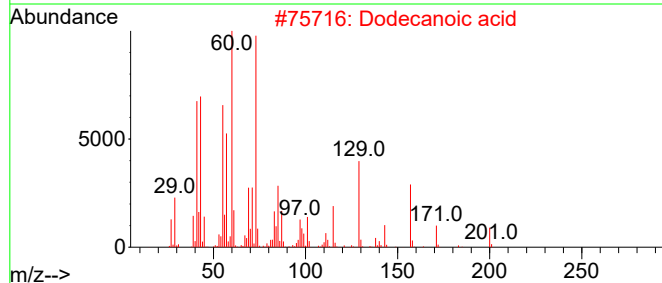
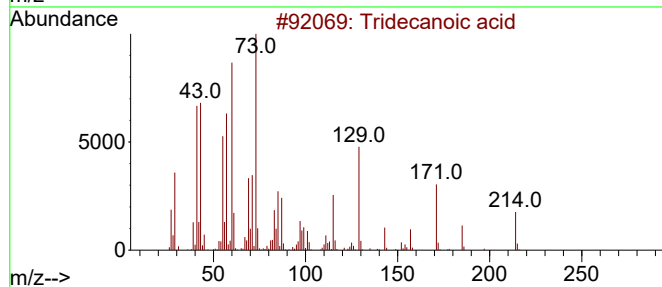
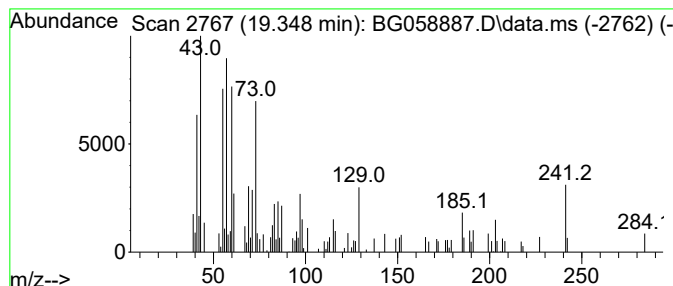
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Tridecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.348	2.74 ng	60754	Chrysene-d12	21.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecanoic acid	214	C13H26O2	000638-53-9	50
2			Dodecanoic acid	200	C12H24O2	000143-07-7	50
3			n-Decanoic acid	172	C10H20O2	000334-48-5	49
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	47
5			Undecanoic acid	186	C11H22O2	000112-37-8	46



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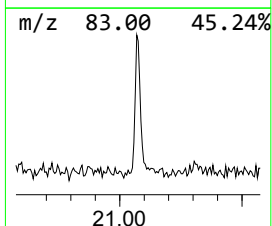
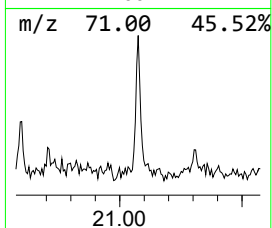
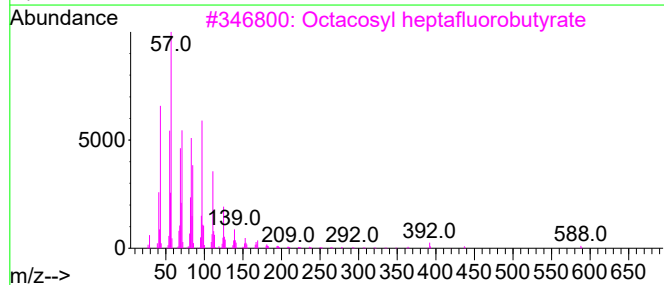
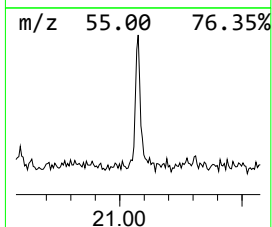
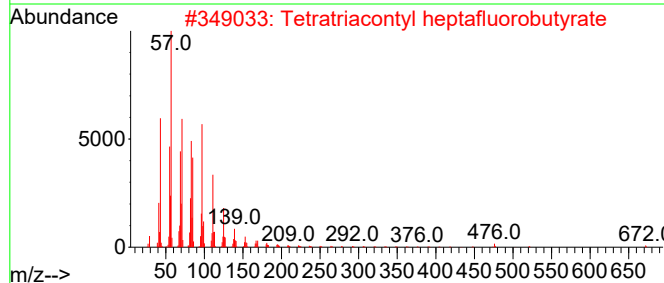
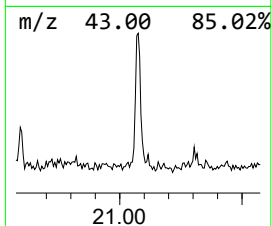
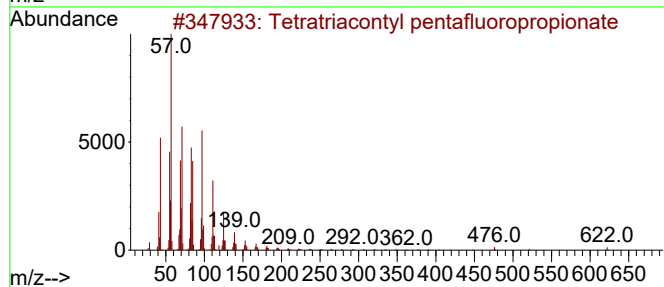
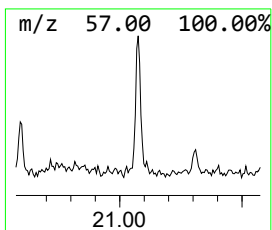
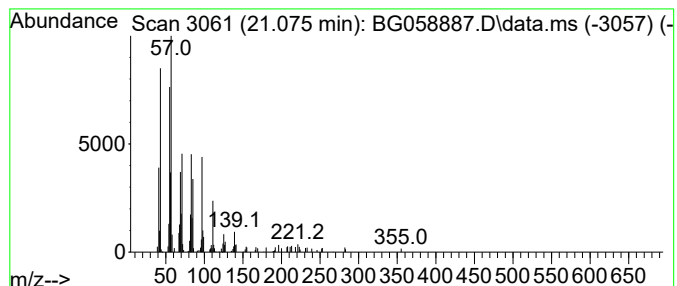
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Tetratriacontyl pentafluoro... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.075	6.61 ng	146721	Chrysene-d12	21.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetratriacontyl pentafluoropropi...	641	C37H69F502	1000351-81-5	91
2			Tetratriacontyl heptafluorobutyrate	691	C38H69F702	1000351-84-1	91
3			Octacosyl heptafluorobutyrate	606	C32H57F702	1010351-83-6	90
4			Pentadecafluorooctanoic acid, oc...	666	C26H37F1502	1000406-04-8	90
5			Dotriacontyl pentafluoropropionate	612	C35H65F502	1010351-81-4	87



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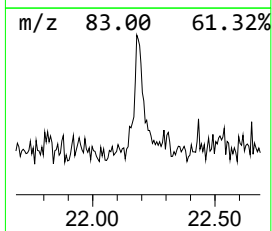
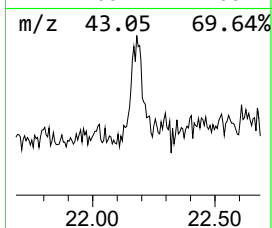
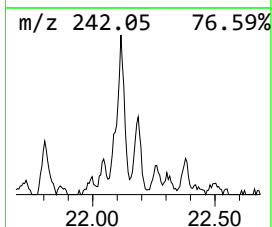
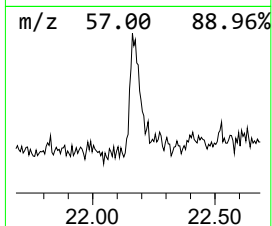
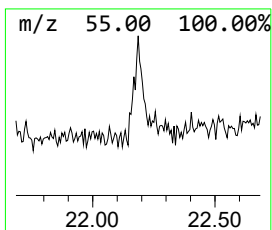
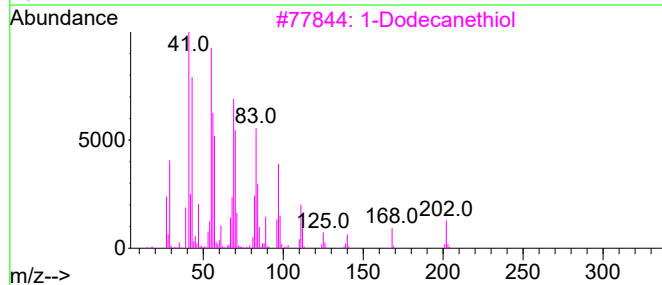
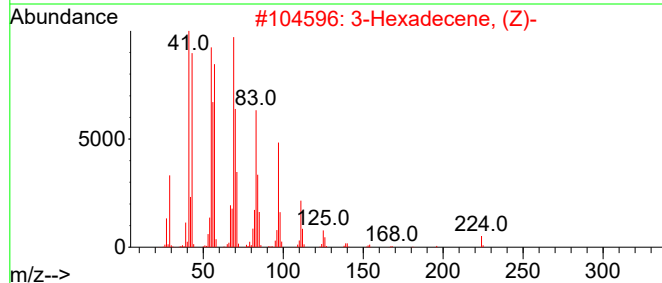
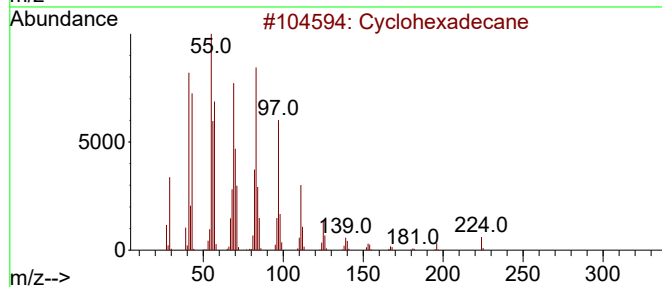
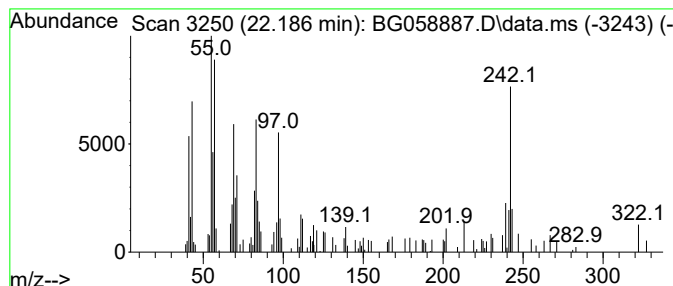
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Cyclohexadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.186	4.23 ng	93759	Chrysene-d12	21.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexadecane	224	C16H32	000295-65-8	93
2			3-Hexadecene, (Z)-	224	C16H32	034303-81-6	55
3			1-Dodecanethiol	202	C12H26S	000112-55-0	55
4			9-Tricosene, (Z)-	322	C23H46	027519-02-4	50
5			Cyclotetradecane	196	C14H28	000295-17-0	46



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG082923\
Data File : BG058887.D
Acq On : 29 Aug 2023 14:42
Operator : MA/JU
Sample : 04165-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
VNJ-210

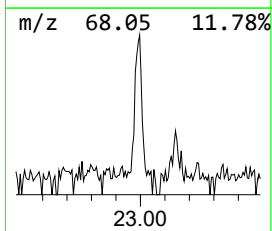
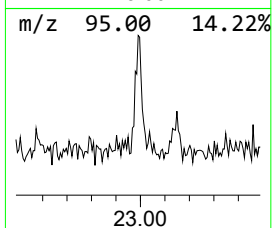
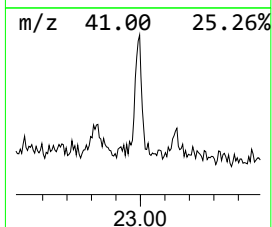
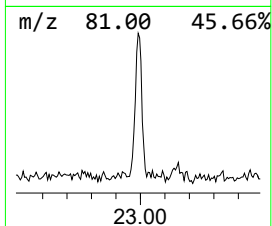
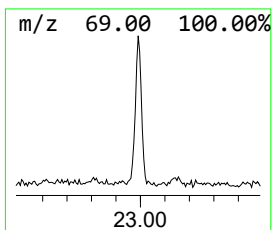
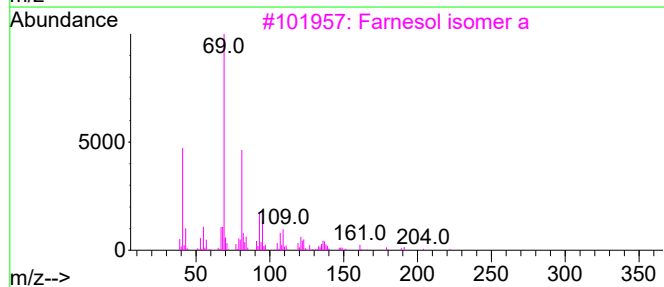
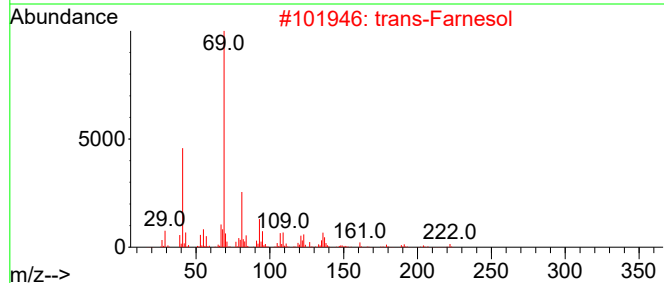
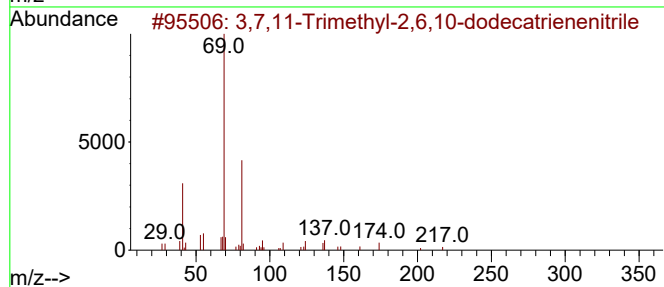
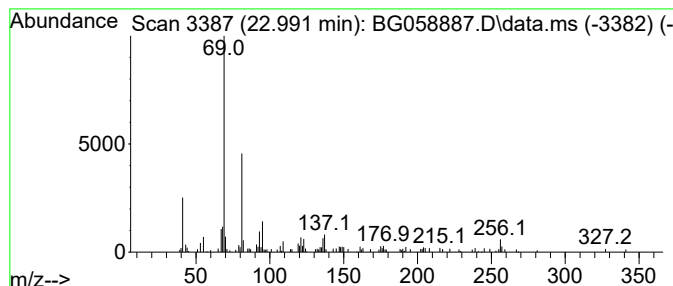
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 3,7,11-Trimethyl-2,6,10-dod... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.991	5.45 ng	100080	Perylene-d12	24.477

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	3,7,11-Trimethyl-2,6,10-dodecatr...	217	C15H23N	029789-67-1	76		
2	trans-Farnesol	222	C15H26O	000106-28-5	76		
3	Farnesol isomer a	222	C15H26O	1000108-92-4	72		
4	2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	004602-84-0	64		
5	(2E,6E,10E)-3,7,11,15-Tetramethy...	318	C21H34O2	125456-63-5	64		



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG082923\
Data File : BG058887.D
Acq On : 29 Aug 2023 14:42
Operator : MA/JU
Sample : 04165-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
VNJ-210

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG081823.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
2,4,7,9-Tetrame...	13.325	5.4	ng	68770	3	14.436	254841	20.0
n-Hexadecanoic ...	18.073	9.7	ng	154004	4	17.186	318482	20.0
Tridecanoic acid	19.348	2.7	ng	60754	5	21.422	443741	20.0
Tetratriacontyl...	21.075	6.6	ng	146721	5	21.422	443741	20.0
Cyclohexadecane	22.186	4.2	ng	93759	5	21.422	443741	20.0
3,7,11-Trimethy...	22.991	5.5	ng	100080	6	24.477	367445	20.0