

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG072822\
 Data File : BG054434.D
 Acq On : 28 Jul 2022 16:26
 Operator : CG/JU
 Sample : N3893-16
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 RVE-16

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-BG071522.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG054434.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.105	15	20	34	rVB	53254	91119	7.53%	1.282%
2	5.566	432	439	450	rVB	189937	326988	27.02%	4.601%
3	7.176	705	713	727	rVB	206080	368903	30.49%	5.191%
4	7.987	843	851	858	rBB	52374	91502	7.56%	1.288%
5	9.150	1041	1049	1060	rVB	129276	236144	19.52%	3.323%
6	10.796	1321	1329	1336	rBV	72074	132593	10.96%	1.866%
7	13.246	1738	1746	1755	rBB	427303	678657	56.09%	9.549%
8	14.626	1974	1981	1988	rBB	130184	206365	17.05%	2.904%
9	16.119	2228	2235	2247	rBV2	404472	655219	54.15%	9.220%
10	17.370	2442	2448	2453	rBV	178349	271401	22.43%	3.819%
11	17.740	2506	2511	2520	rVB4	10331	19234	1.59%	0.271%
12	18.028	2555	2560	2564	rBV	18644	25481	2.11%	0.359%
13	18.146	2574	2580	2584	rBV4	7310	13374	1.11%	0.188%
14	18.199	2586	2589	2594	rBV2	8648	14434	1.19%	0.203%
15	18.257	2594	2599	2604	rBV4	46555	75017	6.20%	1.056%
16	19.162	2748	2753	2755	rBV3	10872	17822	1.47%	0.251%
17	19.192	2755	2758	2766	rVB4	38641	55943	4.62%	0.787%
18	19.421	2788	2797	2804	rVV	44440	96224	7.95%	1.354%
19	19.527	2812	2815	2820	rBV5	11178	15816	1.31%	0.223%
20	19.785	2854	2859	2867	rVB	39673	64176	5.30%	0.903%
21	19.861	2867	2872	2875	rBV5	7985	13029	1.08%	0.183%
22	19.979	2886	2892	2898	rBV	898066	1210038	100.00%	17.027%
23	20.390	2958	2962	2966	rBV4	12970	21236	1.75%	0.299%
24	20.584	2990	2995	2996	rBV3	12104	20842	1.72%	0.293%
25	20.954	3055	3058	3062	rVB5	25579	29804	2.46%	0.419%
26	21.272	3107	3112	3117	rBV2	49258	76287	6.30%	1.073%
27	21.636	3167	3174	3179	rBV	208517	384372	31.77%	5.409%
28	22.053	3242	3245	3259	rVB8	38513	85802	7.09%	1.207%
29	22.441	3304	3311	3318	rVB7	23781	71877	5.94%	1.011%
30	23.451	3478	3483	3492	rVB5	42762	89854	7.43%	1.264%
31	23.892	3556	3558	3565	rVB3	36081	62635	5.18%	0.881%
32	24.838	3711	3719	3729	rVB2	124511	350581	28.97%	4.933%
33	25.954	3903	3909	3918	rVB3	40740	117287	9.69%	1.650%
34	28.992	4411	4426	4443	rVB6	214057	1083936	89.58%	15.252%
35	30.114	4610	4617	4618	rBV7	17094	32766	2.71%	0.461%

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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_G\Methods\8270-BG071522.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

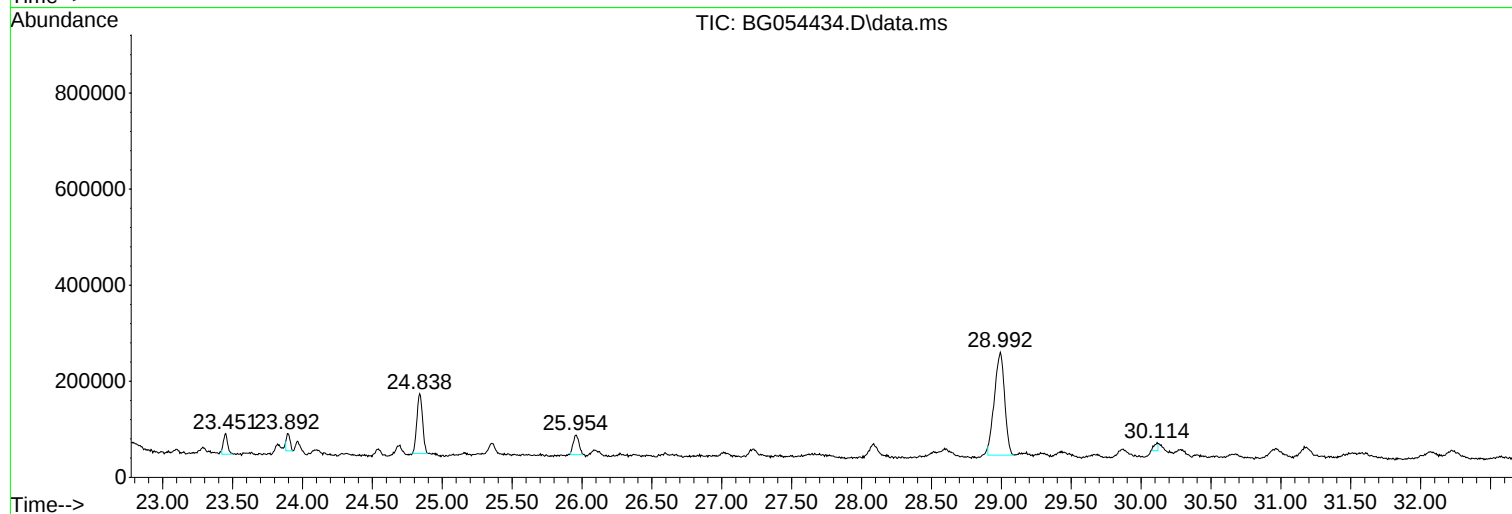
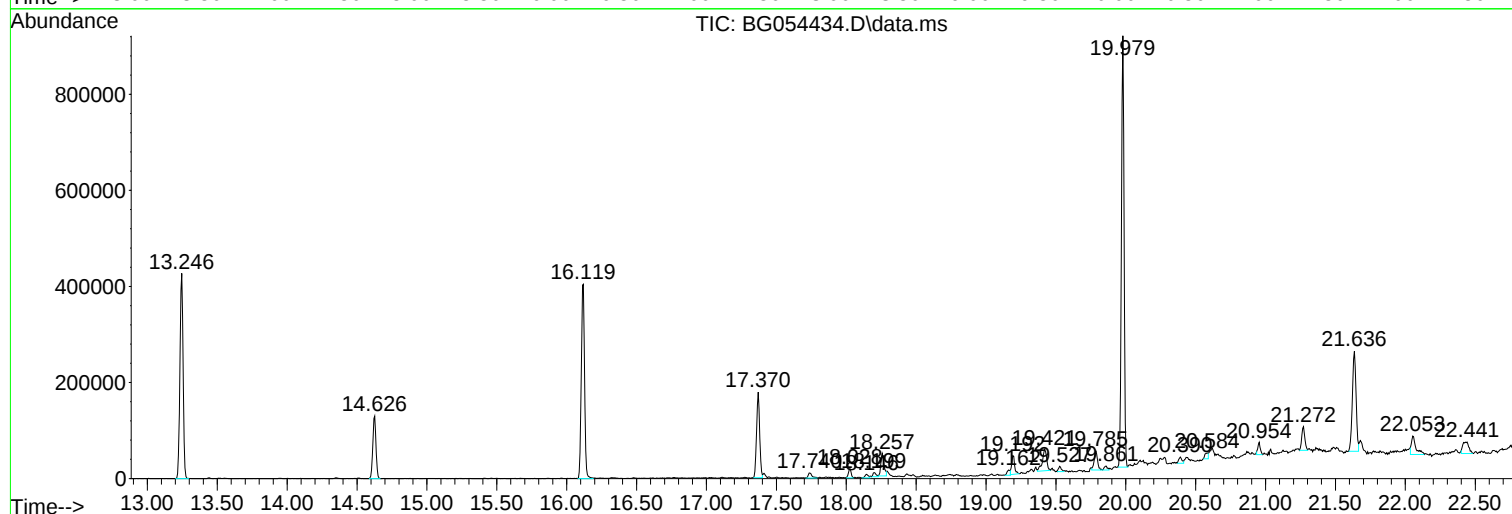
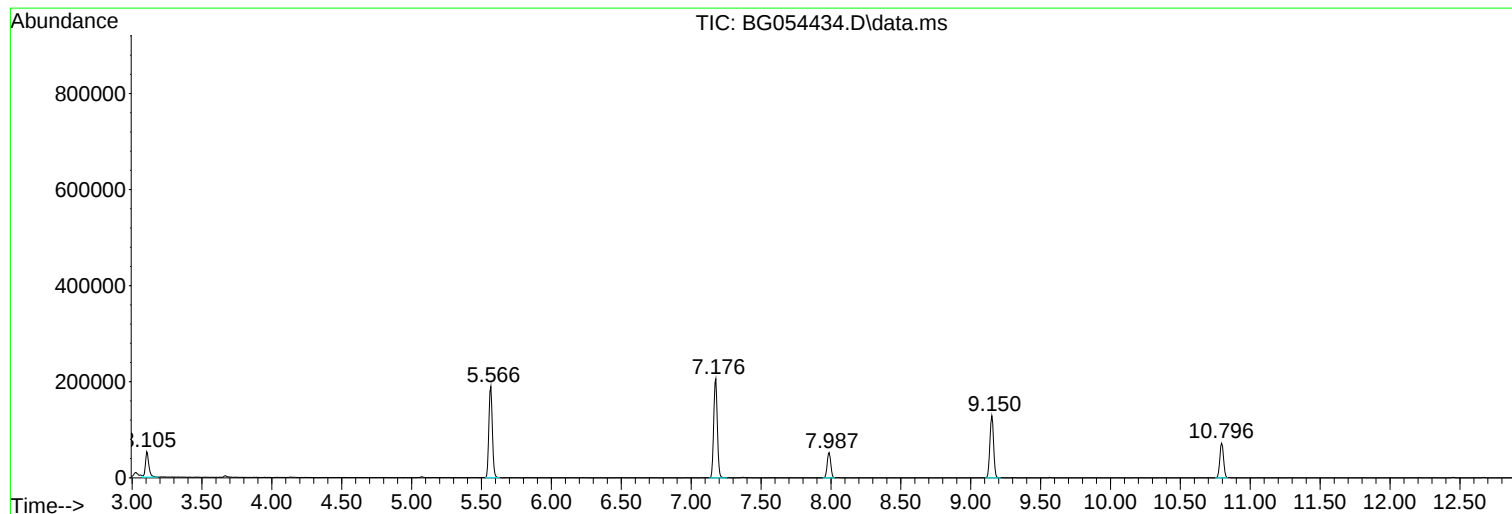
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG071522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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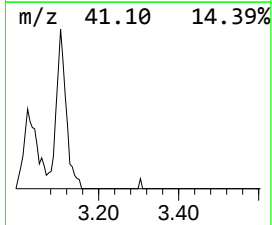
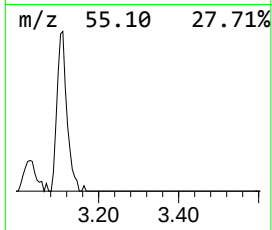
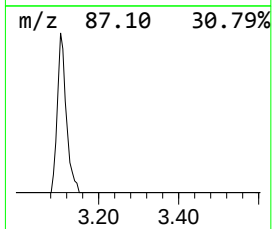
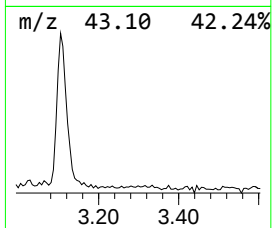
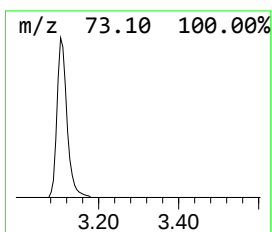
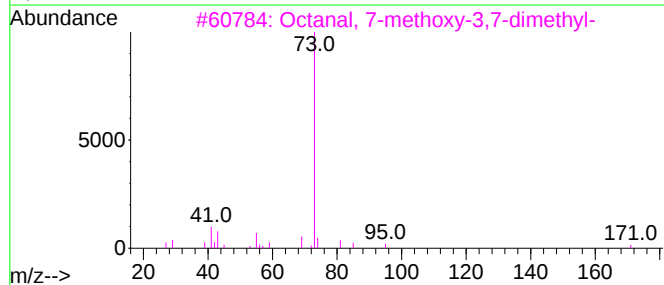
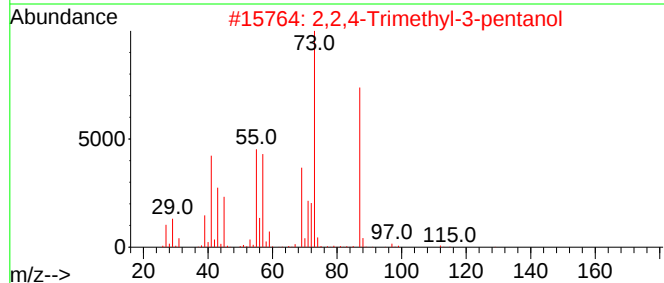
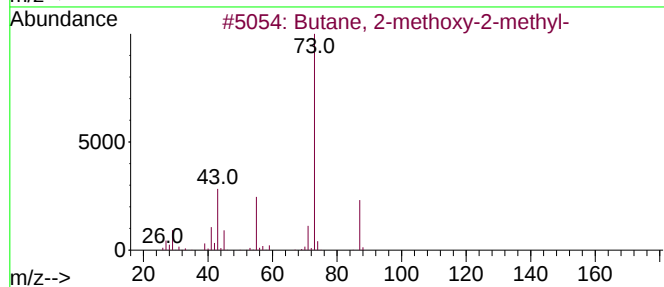
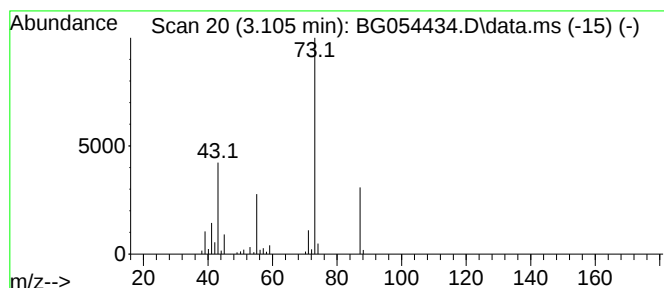
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.105	19.92 ng	91119	1,4-Dichlorobenzene-d4	7.987

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	40
3			Octanal, 7-methoxy-3,7-dimethyl-	186	C11H22O2	003613-30-7	17
4			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	10
5			3-Hexanol, 2,4-dimethyl-	130	C8H18O	013432-25-2	9



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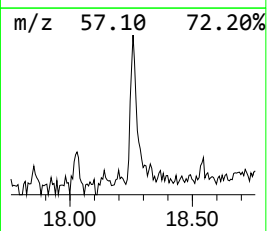
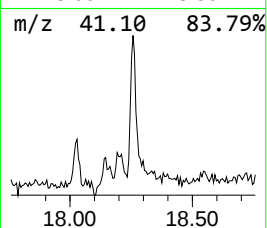
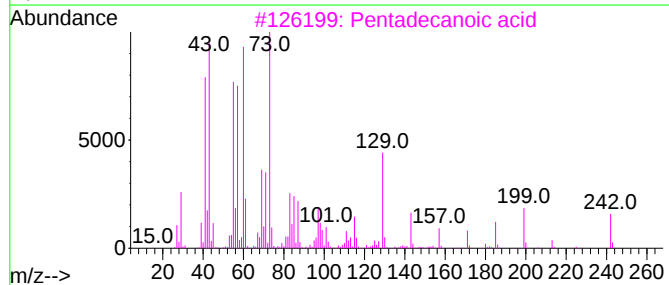
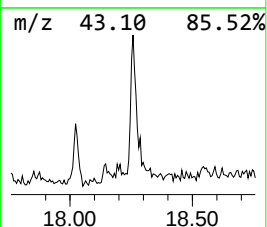
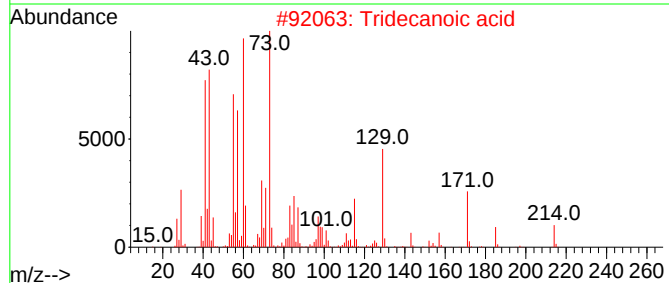
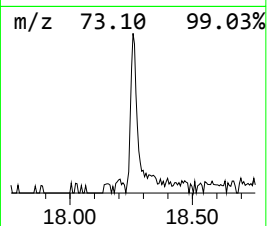
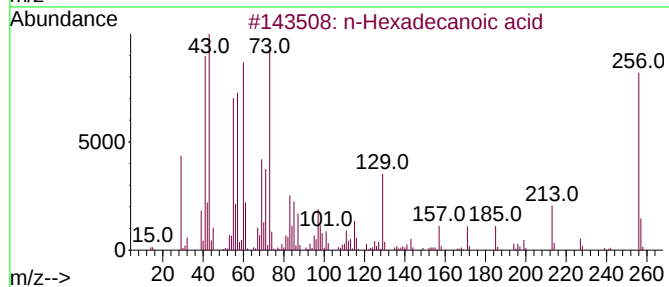
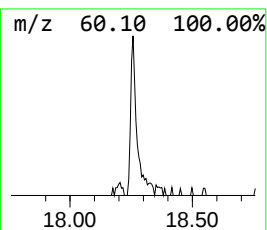
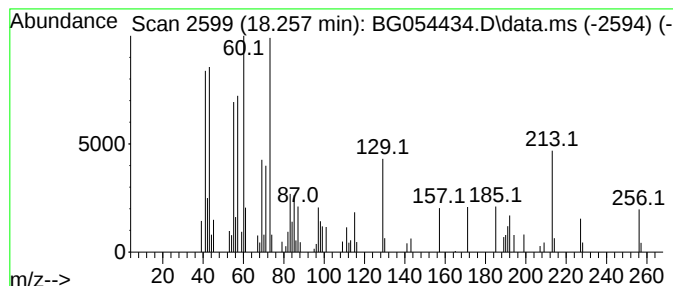
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG071522.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.257	5.53 ng	75017	Phenanthrene-d10	17.370

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2			Tridecanoic acid	214	C13H26O2	000638-53-9	91
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	53
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	49
5			Dodecanoic acid	200	C12H24O2	000143-07-7	43



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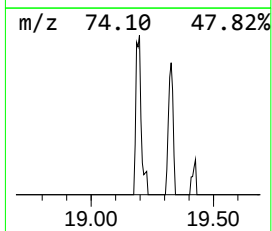
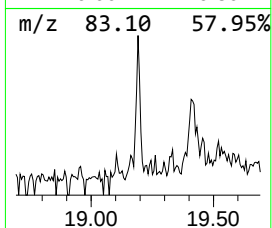
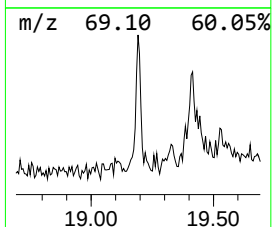
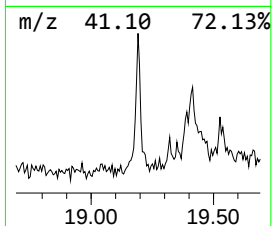
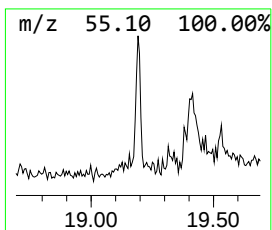
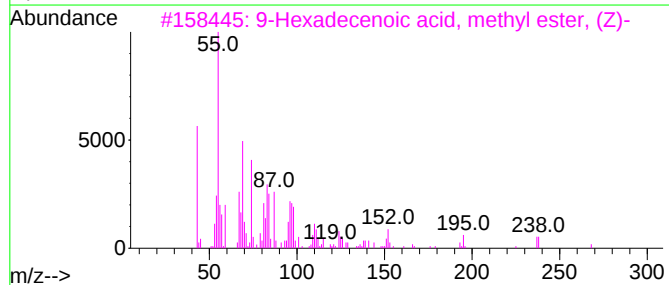
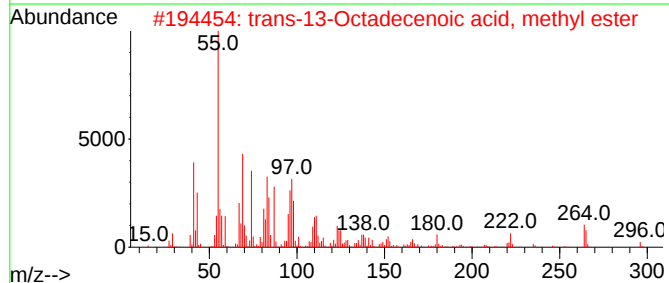
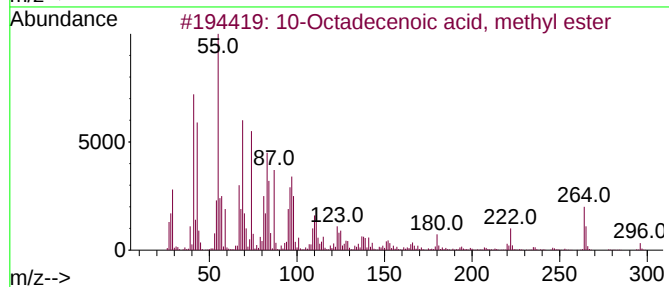
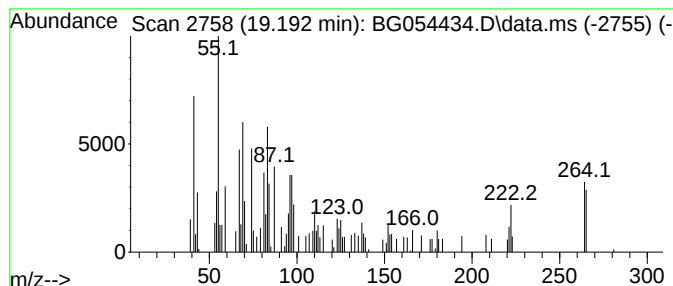
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 10-Octadecenoic acid, methy... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.192	4.12 ng	55943	Phenanthrene-d10	17.370

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	80
2			trans-13-Octadecenoic acid, meth...	296	C19H36O2	1000333-61-3	64
3			9-Hexadecenoic acid, methyl este...	268	C17H32O2	001120-25-8	58
4			Methyl (Z)-10-pentadecenoate	254	C16H30O2	1000426-92-2	52
5			7-Hexadecenoic acid, methyl este...	268	C17H32O2	056875-67-3	49



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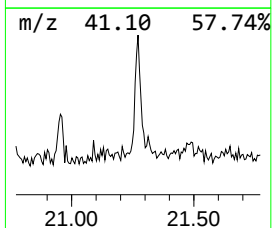
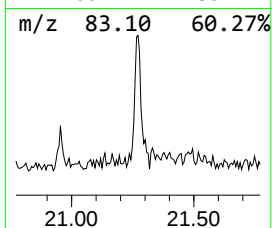
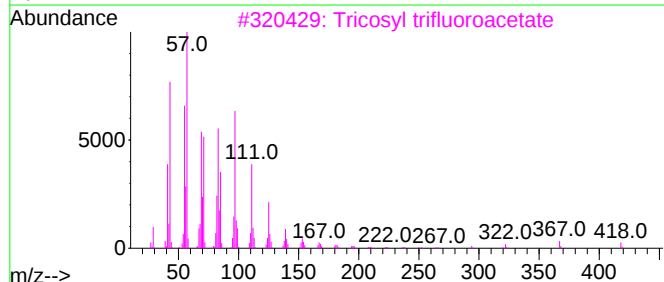
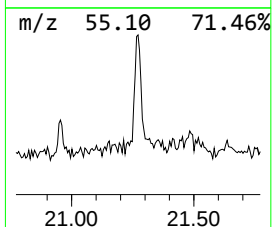
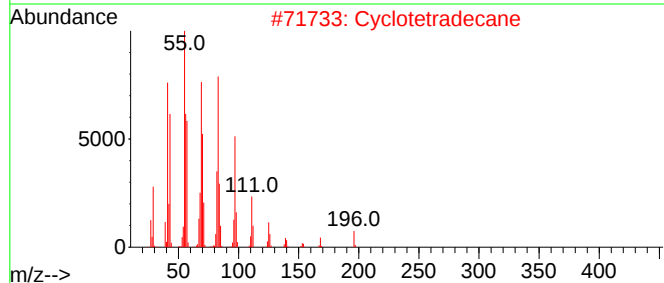
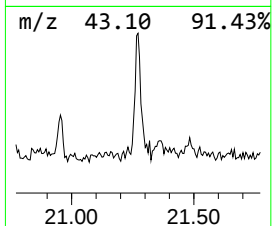
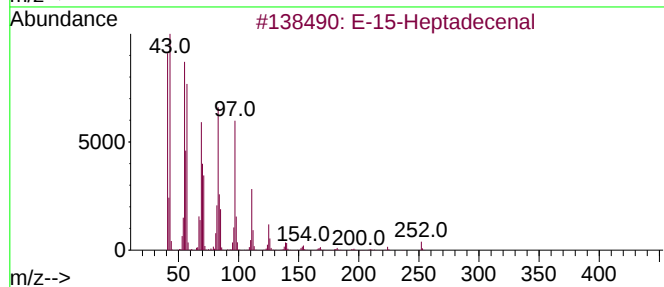
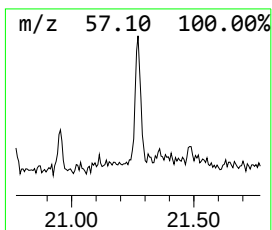
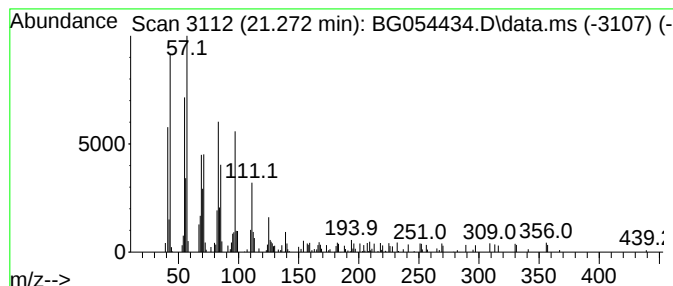
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 E-15-Heptadecenal Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.272	3.97 ng	76287	Chrysene-d12	21.636

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			E-15-Heptadecenal	252	C17H32O	1000130-97-9	98
2			Cyclotetradecane	196	C14H28	000295-17-0	94
3			Tricosyl trifluoroacetate	436	C25H47F3O2	1000351-75-1	90
4			1-Octadecene	252	C18H36	000112-88-9	87
5			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	81



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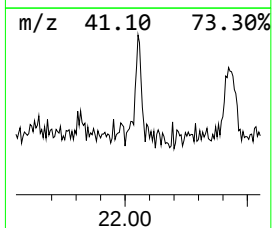
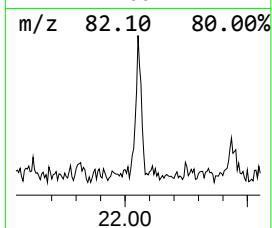
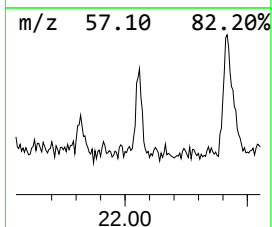
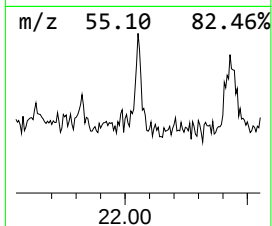
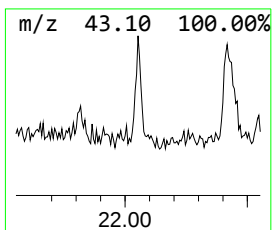
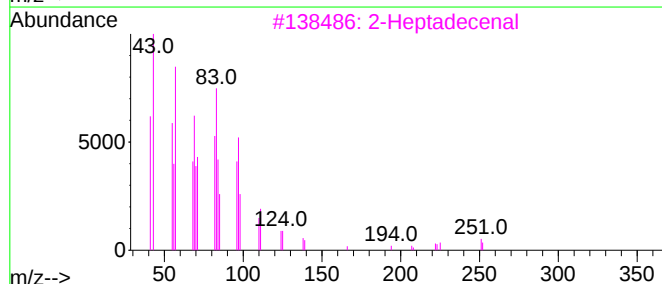
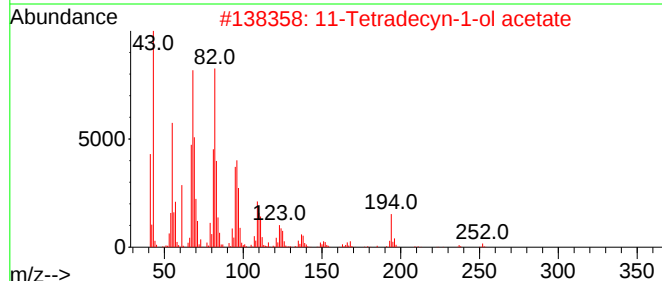
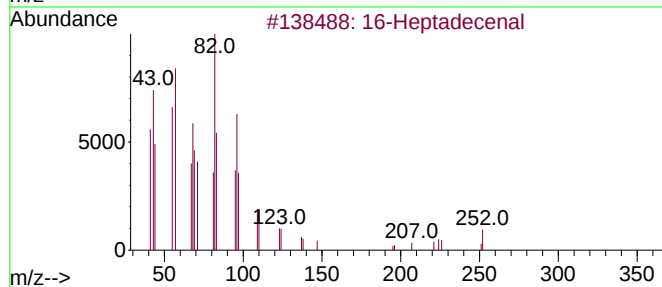
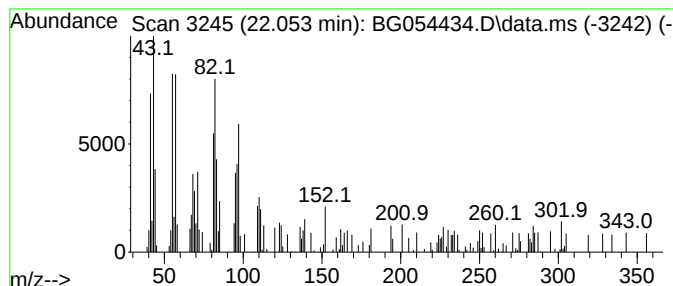
Instrument :
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ClientSampleId :
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 16-Heptadecenal Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
22.053	4.46 ng	85802	Chrysene-d12	21.636	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	16-Heptadecenal	252	C17H32O	1010144-57-9	58
2	11-Tetradecyn-1-ol acetate	252	C16H28O2	033925-72-3	58
3	2-Heptadecenal	252	C17H32O	1000143-48-6	55
4	Bicyclo[4.1.0]heptane, 7-butyl-	152	C11H20	018645-10-8	55
5	Eicosanal-	296	C20H40O	002400-66-0	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG072822\
Data File : BG054434.D
Acq On : 28 Jul 2022 16:26
Operator : CG/JU
Sample : N3893-16
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
RVE-16

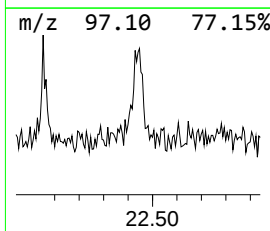
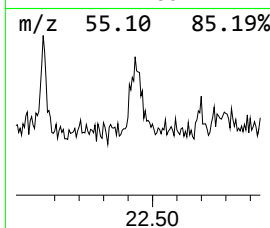
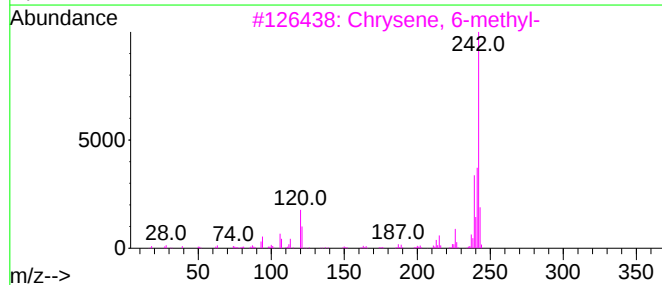
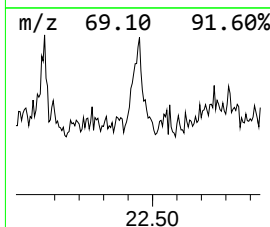
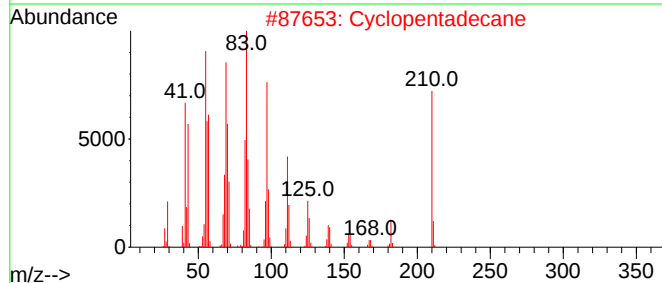
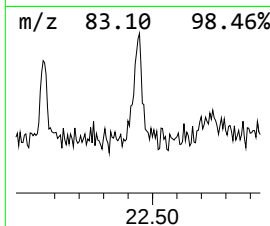
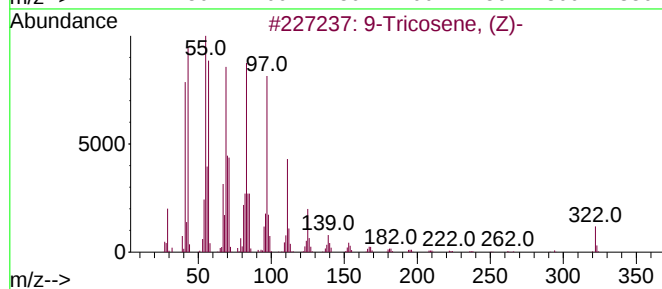
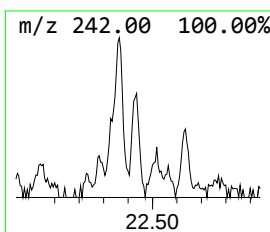
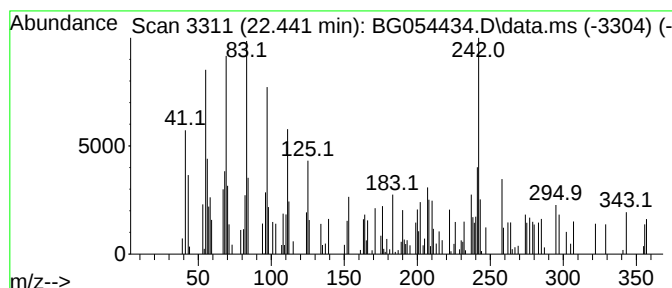
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown22.441 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.441	3.74 ng	71877	Chrysene-d12	21.636

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Tricosene, (Z)-			322	C23H46	027519-02-4	43
2	Cyclopentadecane			210	C15H30	000295-48-7	35
3	Chrysene, 6-methyl-			242	C19H14	001705-85-7	25
4	Chrysene, 5-methyl-			242	C19H14	003697-24-3	25
5	Benz[a]anthracene, 12-methyl-			242	C19H14	002422-79-9	22



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG072822\
Data File : BG054434.D
Acq On : 28 Jul 2022 16:26
Operator : CG/JU
Sample : N3893-16
Misc :
ALS Vial : 10 Sample Multiplier: 1

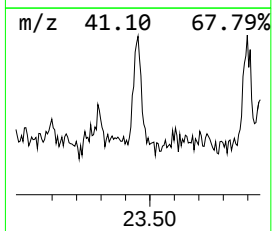
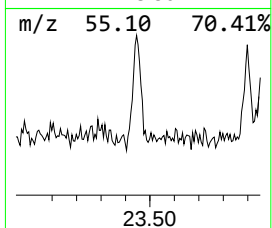
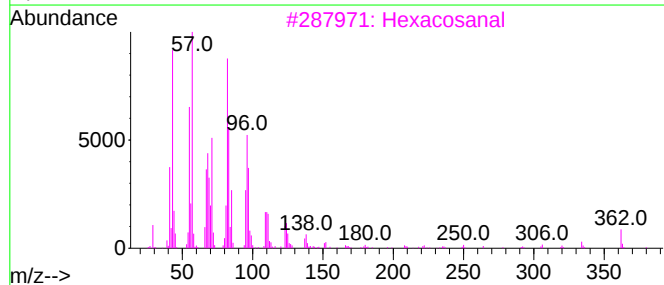
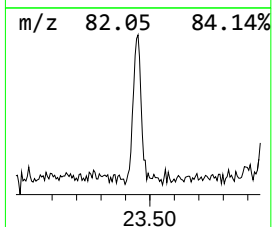
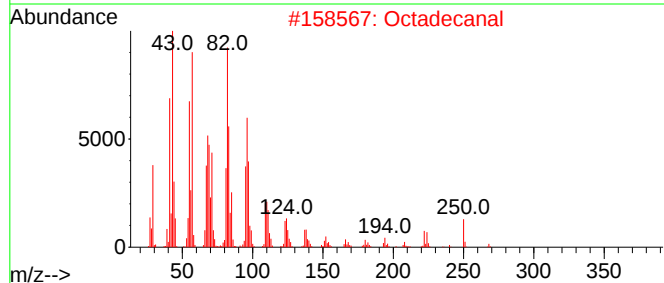
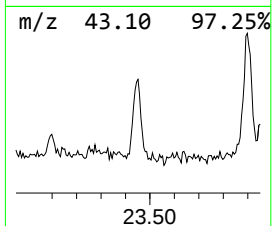
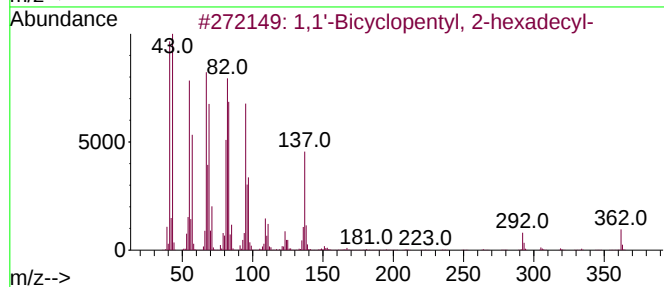
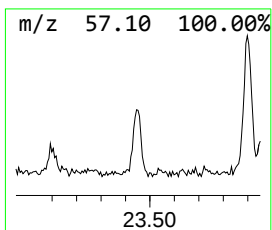
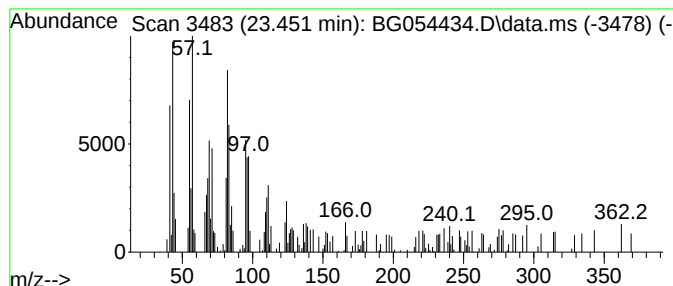
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG071522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 1,1'-Bicyclopentyl, 2-hexad... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.	
23.451	5.13 ng	89854	Perylene-d12		24.838	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	1,1'-Bicyclopentyl, 2-hexadecyl-		362	C26H50	055334-11-7	83
2	Octadecanal		268	C18H36O	000638-66-4	64
3	Hexacosanal		380	C26H52O	026627-85-0	58
4	Tridecanal		198	C13H26O	010486-19-8	58
5	Bicyclo[10.8.0]eicosane, (E)-		278	C20H38	1010155-85-0	58



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG072822\
Data File : BG054434.D
Acq On : 28 Jul 2022 16:26
Operator : CG/JU
Sample : N3893-16
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
RVE-16

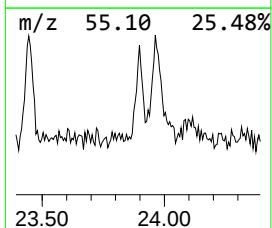
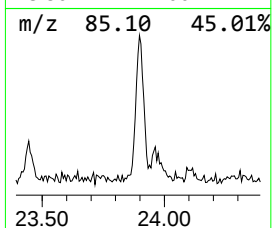
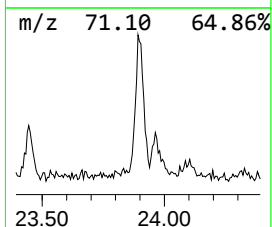
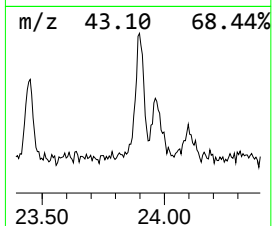
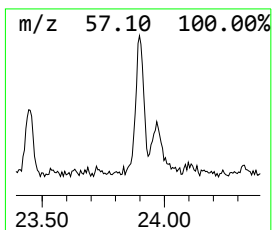
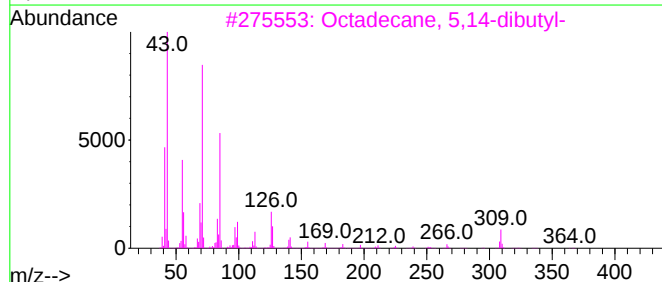
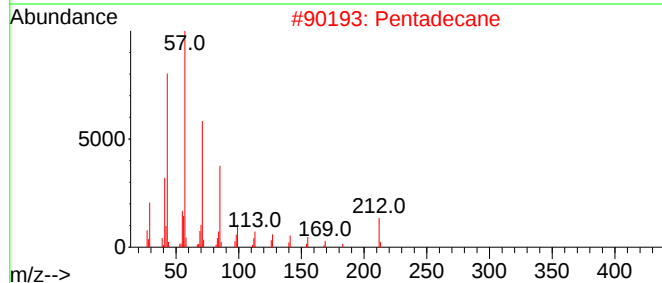
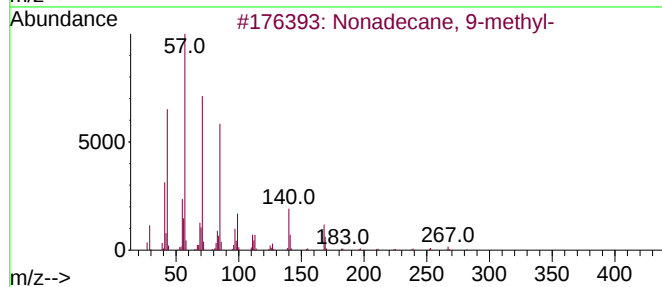
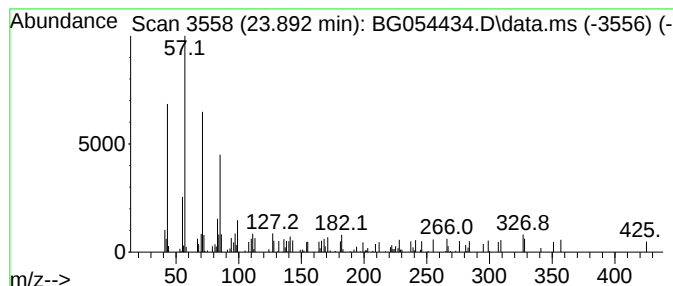
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Nonadecane, 9-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.892	3.57 ng	62635	Perylene-d12	24.838

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonadecane, 9-methyl-	282	C20H42	013287-24-6	83
2			Pentadecane	212	C15H32	000629-62-9	64
3			Octadecane, 5,14-dibutyl-	366	C26H54	055282-13-8	62
4			Heneicosane, 11-decyl-	437	C31H64	055320-06-4	58
5			Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG072822\
Data File : BG054434.D
Acq On : 28 Jul 2022 16:26
Operator : CG/JU
Sample : N3893-16
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
RVE-16

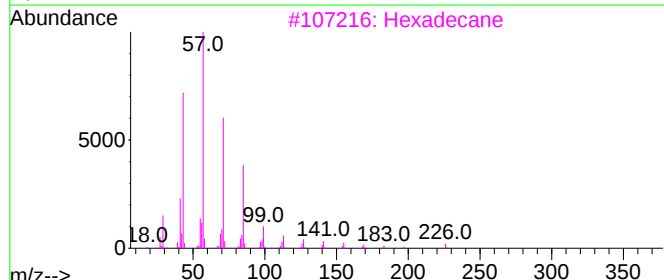
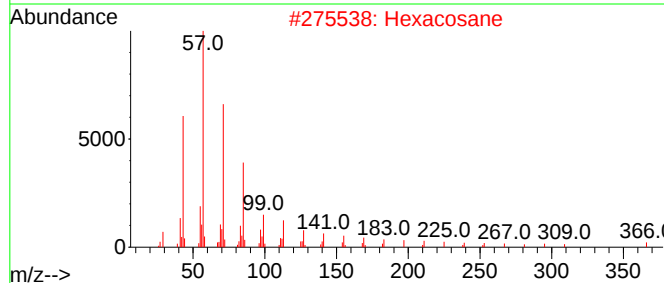
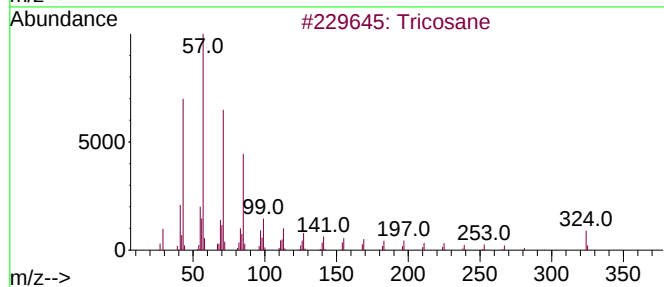
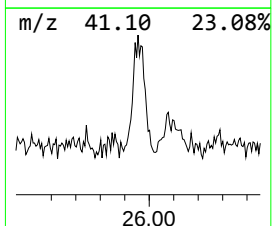
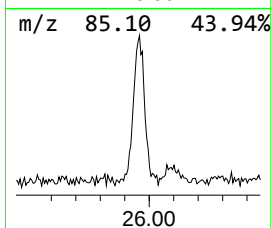
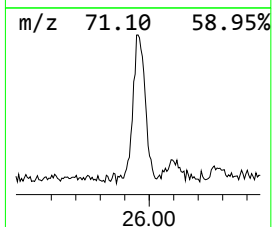
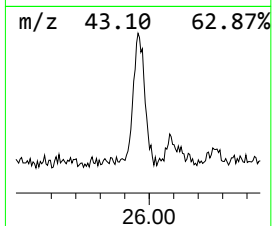
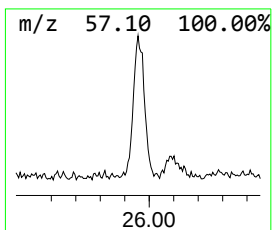
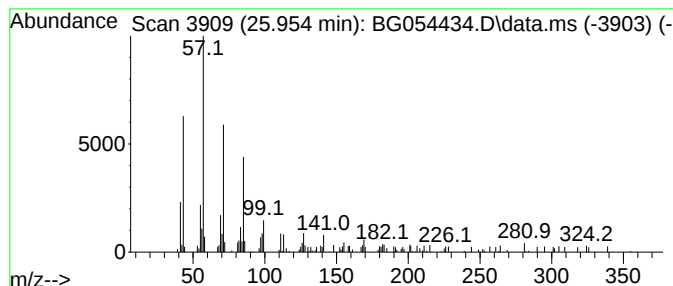
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Tricosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.954	6.69 ng	117287	Perylene-d12	24.838

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tricosane	324	C23H48	000638-67-5	95
2			Hexacosane	366	C26H54	000630-01-3	90
3			Hexadecane	226	C16H34	000544-76-3	87
4			Heneicosane	296	C21H44	000629-94-7	83
5			Octadecane	254	C18H38	000593-45-3	83



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG072822\
Data File : BG054434.D
Acq On : 28 Jul 2022 16:26
Operator : CG/JU
Sample : N3893-16
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
RVE-16

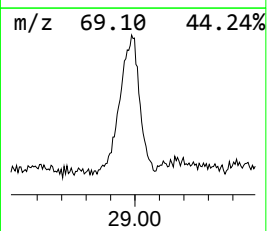
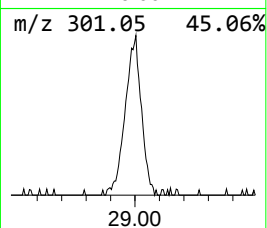
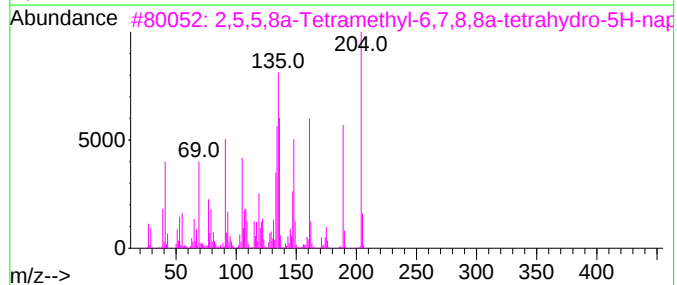
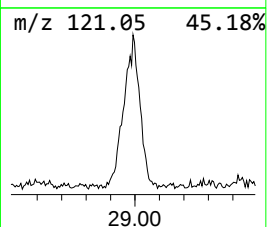
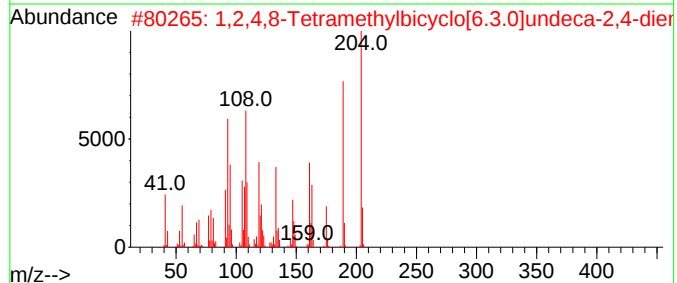
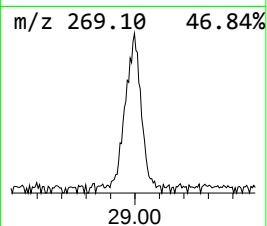
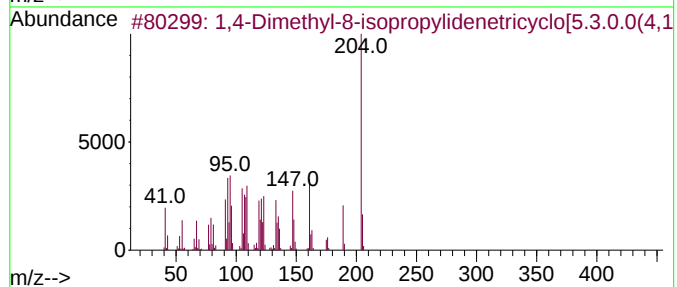
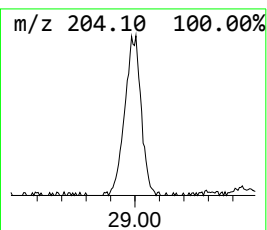
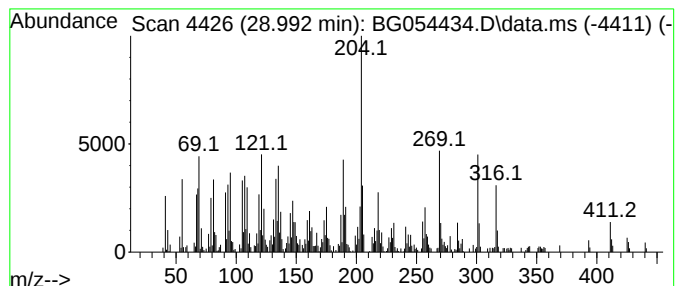
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 unknown28.992 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
28.992	61.84 ng	1083940	Perylene-d12	24.838

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,4-Dimethyl-8-isopropylidenetri...	204	C15H24	1010140-07-7	49
2			1,2,4,8-Tetramethylbicyclo[6.3.0...	204	C15H24	137235-51-9	41
3			2,5,5,8a-Tetramethyl-6,7,8,8a-te...	204	C14H20O	124957-09-1	38
4			1,1,4a-Trimethyl-5,6-dimethylene...	204	C15H24	1000193-60-8	38
5			3-Chloro-5-fluoro-4-methoxybenzo...	204	C8H6ClFO3	886497-22-9	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG072822\
Data File : BG054434.D
Acq On : 28 Jul 2022 16:26
Operator : CG/JU
Sample : N3893-16
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
RVE-16

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG071522.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
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n-Hexadecanoic ...	18.257	5.5	ng	75017	4	17.370	271401	20.0
10-Octadecenoic...	19.192	4.1	ng	55943	4	17.370	271401	20.0
E-15-Heptadecenal	21.272	4.0	ng	76287	5	21.636	384372	20.0
16-Heptadecenal	22.053	4.5	ng	85802	5	21.636	384372	20.0
unknown22.441	22.441	3.7	ng	71877	5	21.636	384372	20.0
1,1'-Bicyclopen...	23.451	5.1	ng	89854	6	24.838	350581	20.0
Nonadecane, 9-m...	23.892	3.6	ng	62635	6	24.838	350581	20.0
Tricosane	25.954	6.7	ng	117287	6	24.838	350581	20.0
unknown28.992	28.992	61.8	ng	1083940	6	24.838	350581	20.0