

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG121823\
 Data File : BG060070.D
 Acq On : 18 Dec 2023 17:33
 Operator : MA/JU
 Sample : 05796-03
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 RT-SB-06-12-13

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-BG121323.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG060070.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.140	5	9	21	rVB	94357	170169	2.97%	0.712%
2	4.462	228	234	242	rBV	129791	207288	3.61%	0.867%
3	5.068	330	337	347	rBV	1712040	2632247	45.87%	11.006%
4	7.112	678	685	693	rBV	613172	1026076	17.88%	4.290%
5	7.958	821	829	836	rBV	268671	456582	7.96%	1.909%
6	9.116	1018	1026	1035	rBV	566626	992666	17.30%	4.150%
7	10.761	1298	1306	1312	rBV	361877	652202	11.37%	2.727%
8	13.217	1717	1724	1734	rVB	2102287	3101330	54.04%	12.967%
9	13.417	1751	1758	1764	rBV3	56272	96241	1.68%	0.402%
10	14.492	1936	1941	1947	rBV3	94969	154947	2.70%	0.648%
11	14.598	1950	1959	1965	rBV	642350	1038988	18.11%	4.344%
12	14.985	2021	2025	2030	rVB2	48898	74085	1.29%	0.310%
13	15.438	2099	2102	2108	rVB	85806	117762	2.05%	0.492%
14	15.638	2131	2136	2142	rBV3	57251	98131	1.71%	0.410%
15	15.849	2168	2172	2177	rVB3	44608	67502	1.18%	0.282%
16	16.301	2245	2249	2257	rBV	135844	275278	4.80%	1.151%
17	17.101	2382	2385	2390	rVV2	115913	147686	2.57%	0.617%
18	17.153	2391	2394	2399	rVB3	57295	75763	1.32%	0.317%
19	17.341	2421	2426	2430	rBV	909172	1381343	24.07%	5.776%
20	17.388	2430	2434	2439	rVB	380951	582738	10.15%	2.437%
21	17.477	2445	2449	2452	rVB2	102096	119367	2.08%	0.499%
22	17.841	2507	2511	2516	rBV	168320	228487	3.98%	0.955%
23	18.534	2625	2629	2633	rBV3	194561	282168	4.92%	1.180%
24	19.163	2734	2736	2740	rVB	174142	163748	2.85%	0.685%
25	19.398	2772	2776	2782	rBV	601332	837094	14.59%	3.500%
26	19.762	2836	2838	2843	rVB	439129	526354	9.17%	2.201%
27	19.968	2868	2873	2879	rVB	4396370	5738446	100.00%	23.993%
28	21.619	3149	3154	3158	rVB2	891617	1413521	24.63%	5.910%
29	24.815	3694	3698	3706	rVB	569461	1258666	21.93%	5.263%

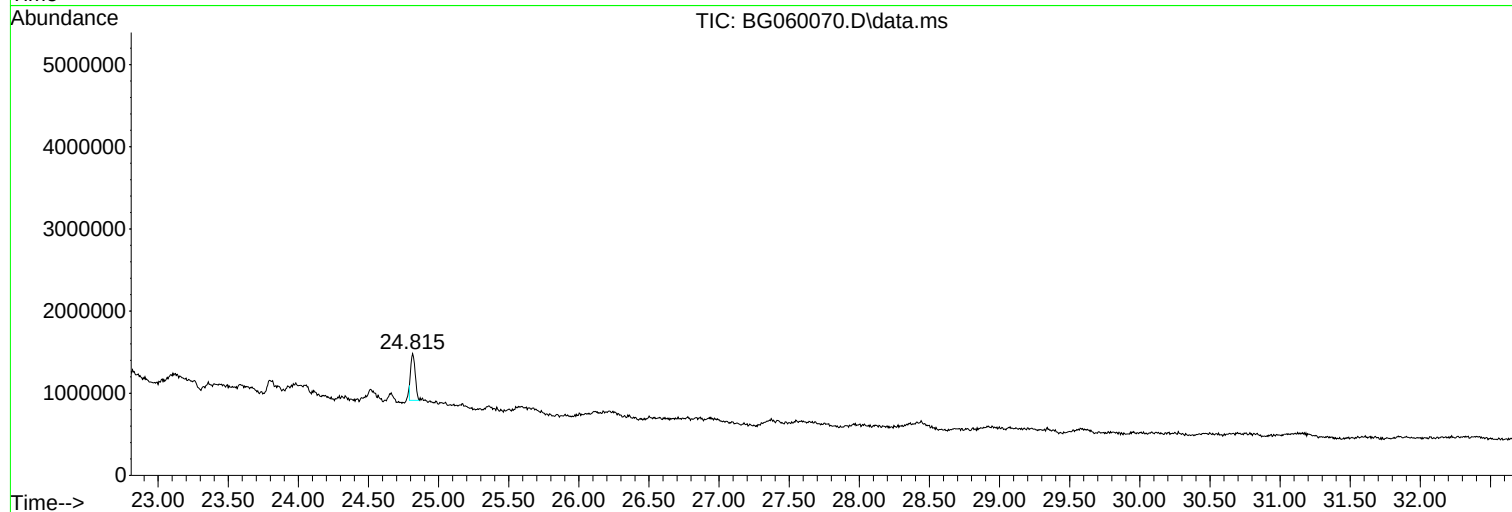
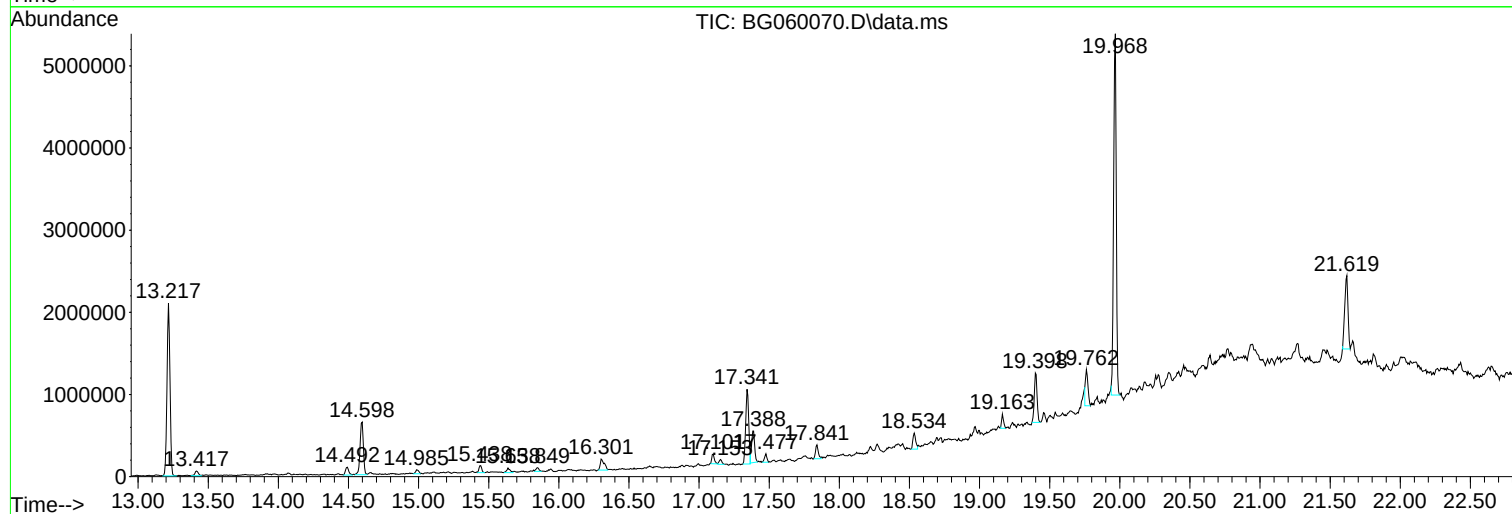
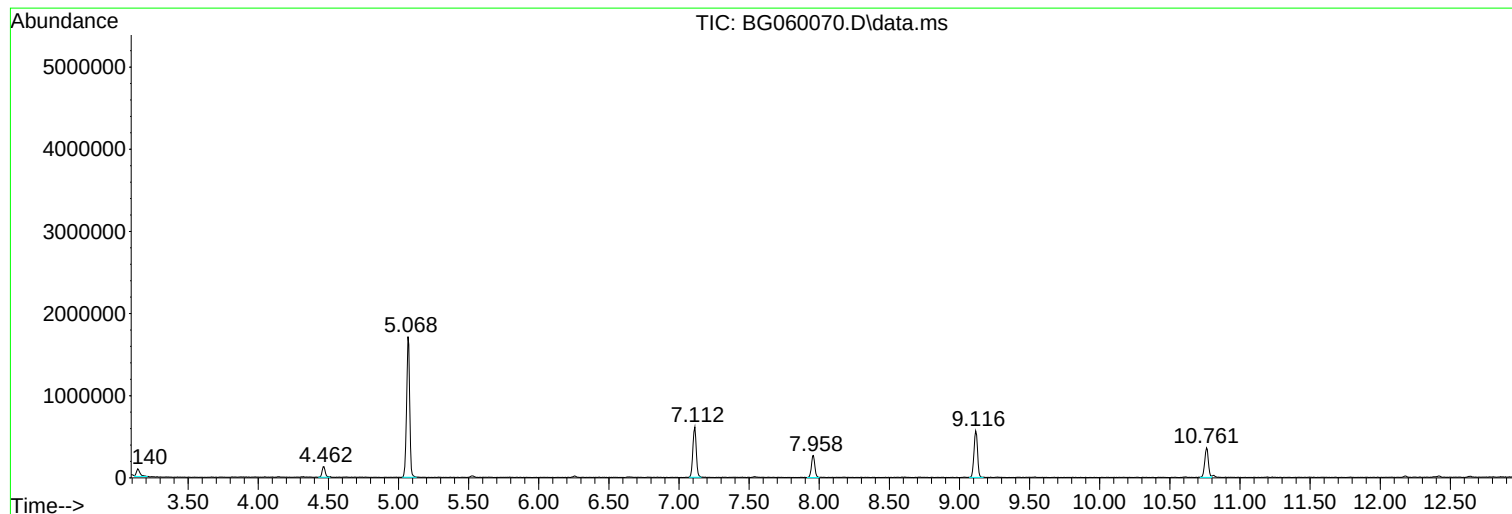
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121323.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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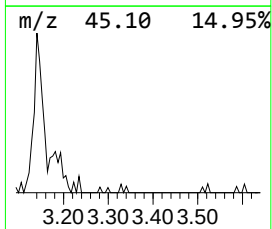
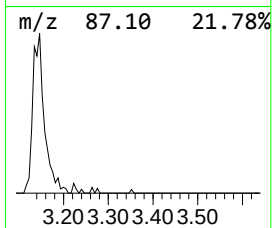
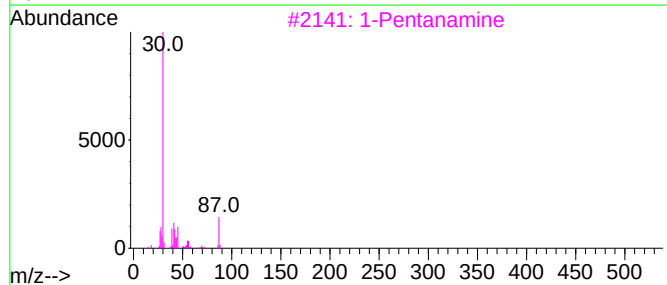
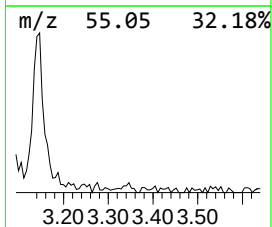
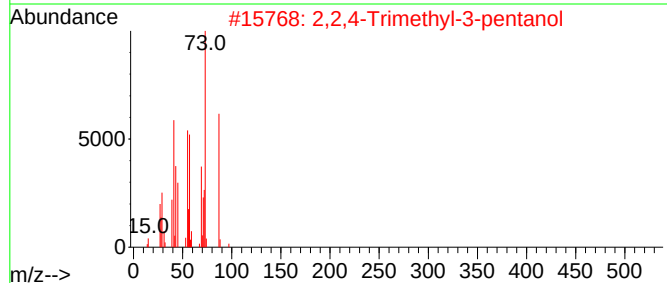
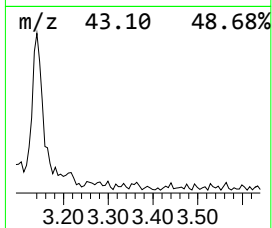
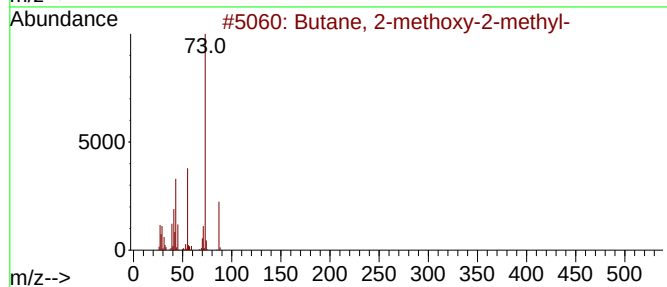
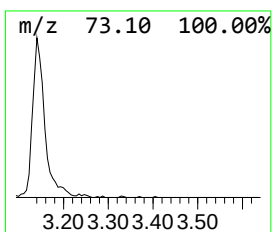
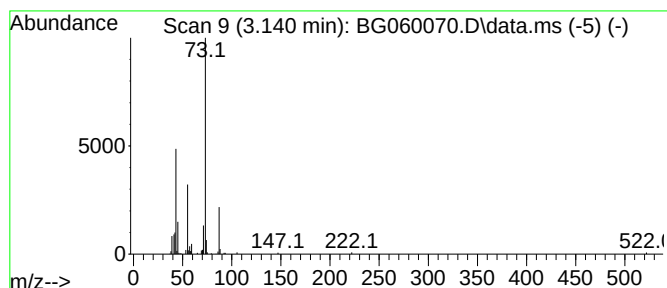
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.140	7.45 ng	170169	1,4-Dichlorobenzene-d4	7.952

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	72
2		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3		1-Pentanamine	87	C5H13N	000110-58-7	32
4		3-Pentanol, 3-methyl-	102	C6H14O	000077-74-7	32
5		1-Propene-1-thiol	74	C3H6S	000925-89-3	23



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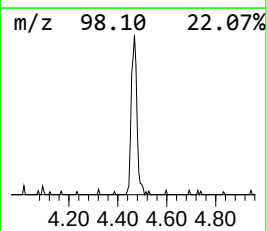
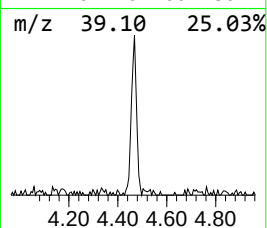
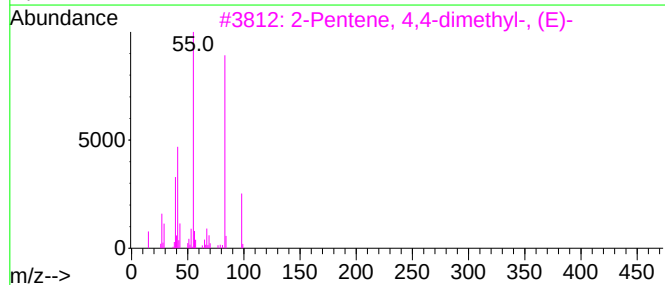
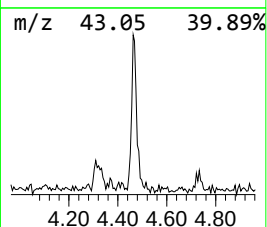
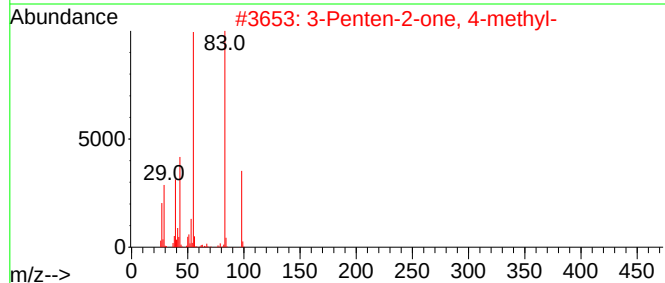
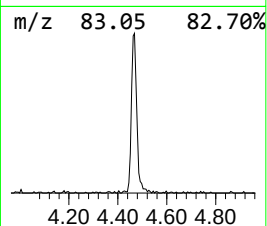
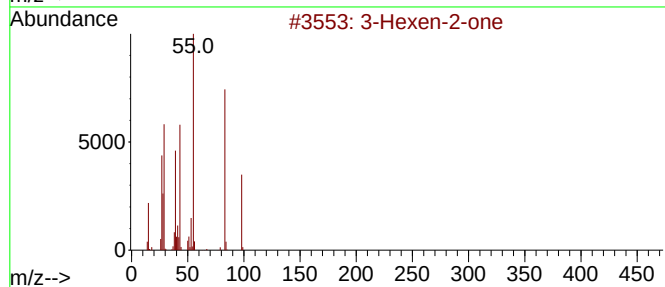
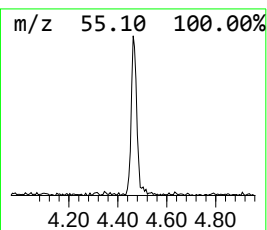
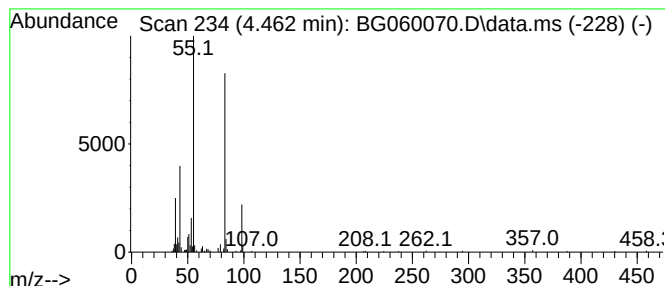
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121323.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 3-Hexen-2-one Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.462	9.08 ng	207288	1,4-Dichlorobenzene-d4	7.952

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Hexen-2-one	98	C6H10O	000763-93-9	87
2			3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	87
3			2-Pentene, 4,4-dimethyl-, (E)-	98	C7H14	000690-08-4	86
4			2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	86
5			2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86



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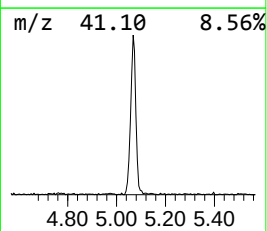
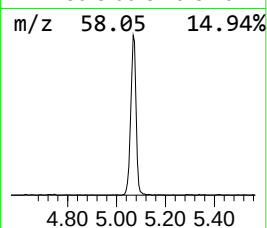
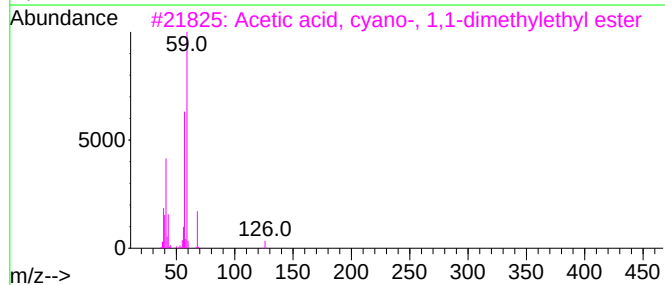
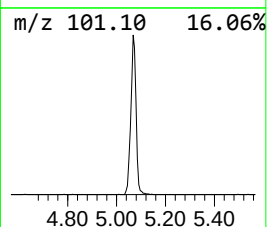
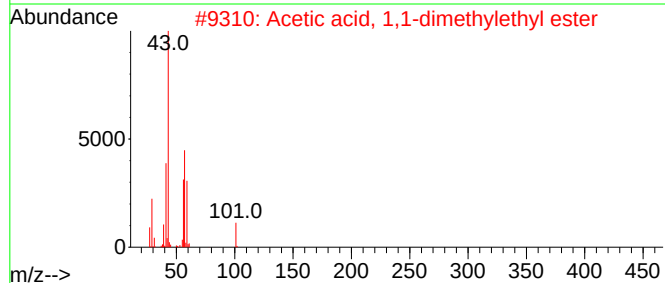
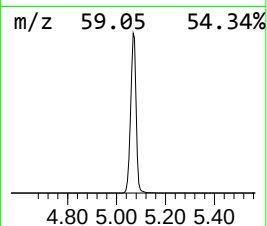
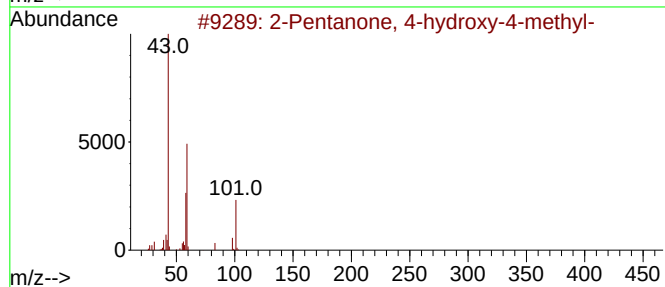
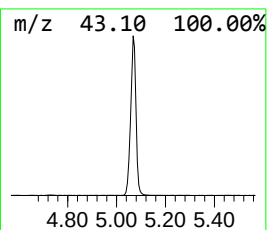
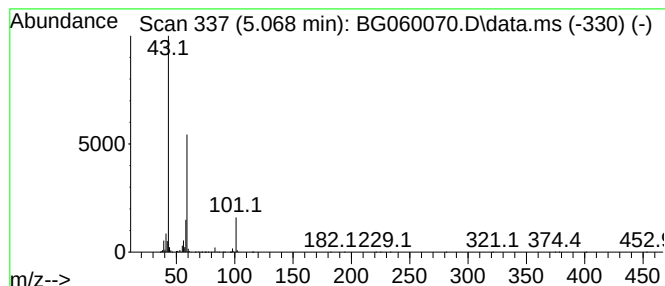
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.068	115.30 ng	2632250	1,4-Dichlorobenzene-d4	7.952

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72	
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	32	
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25	
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	25	
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16	



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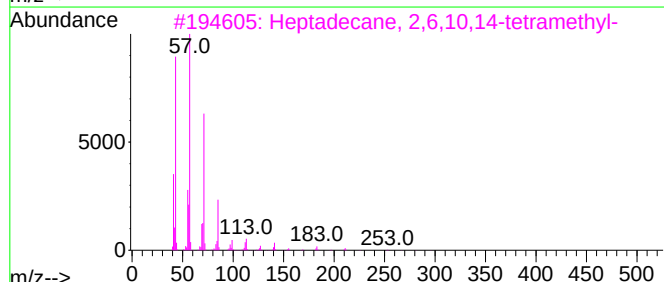
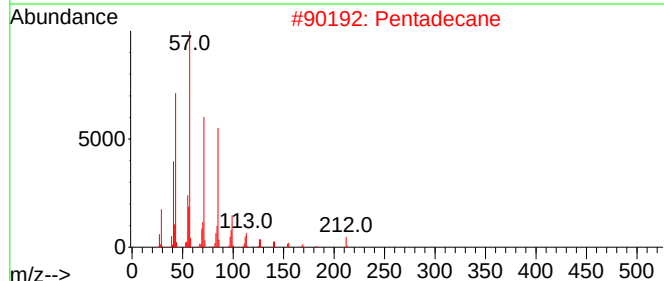
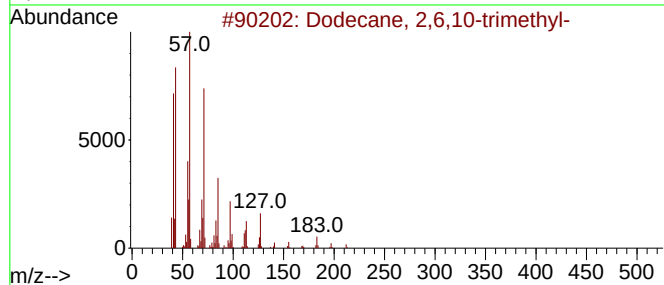
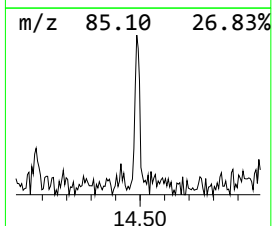
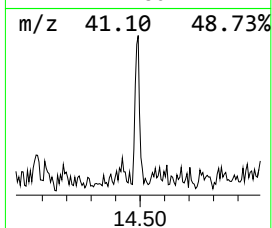
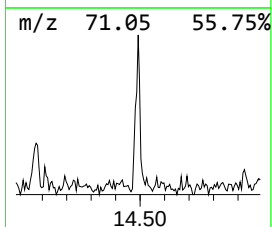
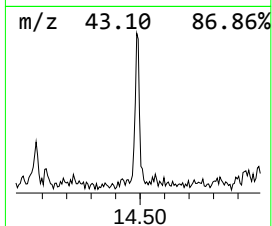
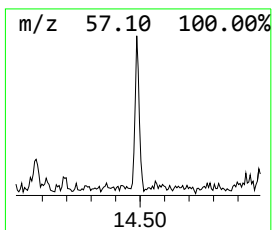
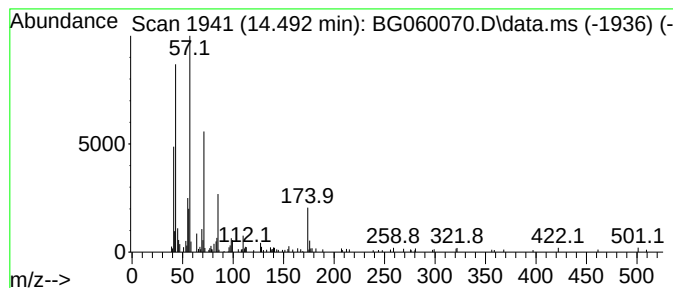
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Peak Number 4 Dodecane, 2,6,10-trimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.492	2.98 ng	154947	Acenaphthene-d10	14.598

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecane, 2,6,10-trimethyl-	212	C15H32	003891-98-3	64
2			Pentadecane	212	C15H32	000629-62-9	64
3			Heptadecane, 2,6,10,14-tetramethyl-	296	C21H44	018344-37-1	64
4			Tridecane	184	C13H28	000629-50-5	59
5			Dodecane, 2-methyl-6-propyl-	226	C16H34	055045-08-4	50



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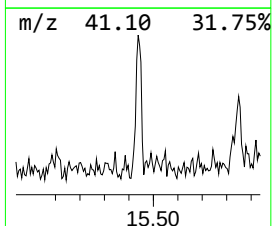
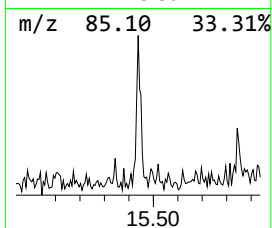
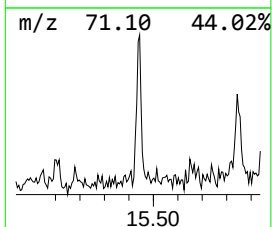
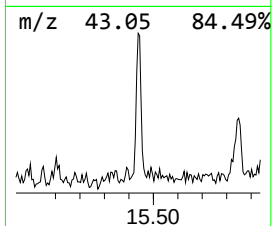
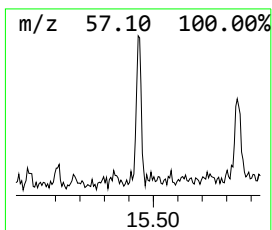
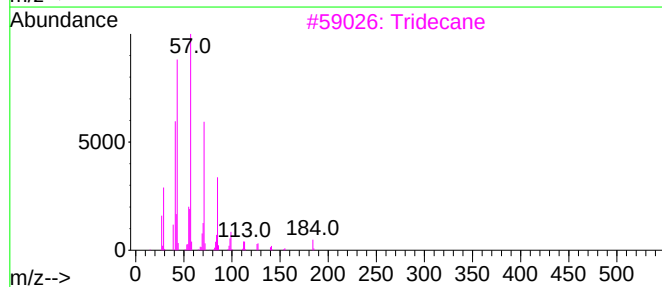
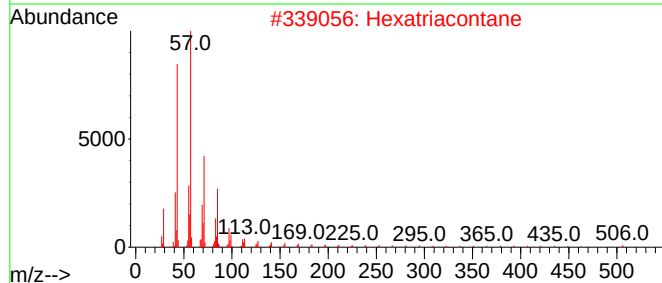
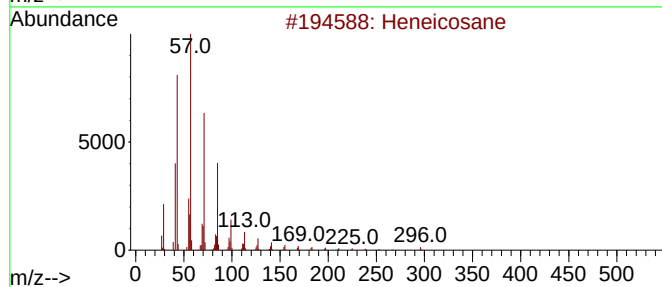
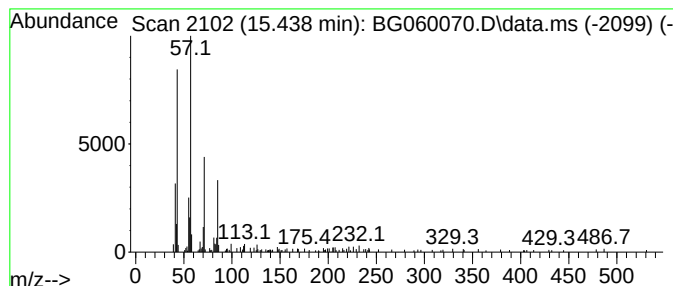
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 Heneicosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.438	2.27 ng	117762	Acenaphthene-d10	14.598

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heneicosane	296	C21H44	000629-94-7	81
2			Hexatriacontane	507	C36H74	000630-06-8	72
3			Tridecane	184	C13H28	000629-50-5	64
4			Undecane, 5,7-dimethyl-	184	C13H28	017312-83-3	64
5			Pentadecane	212	C15H32	000629-62-9	64



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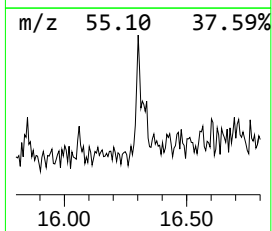
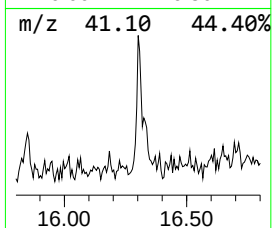
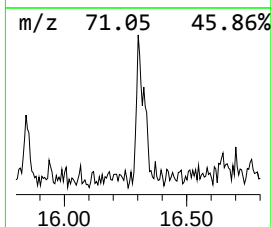
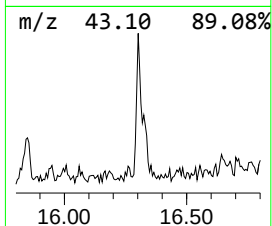
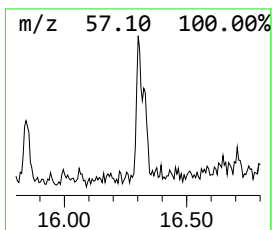
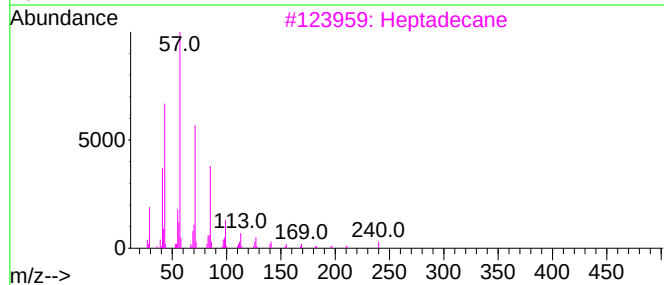
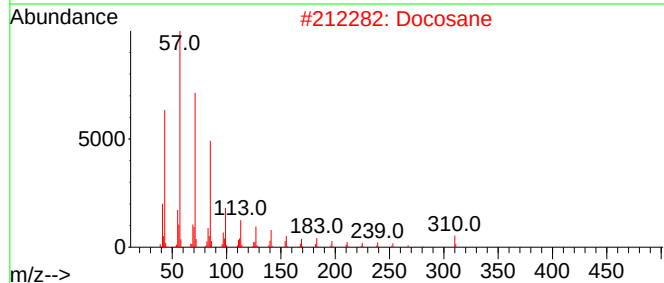
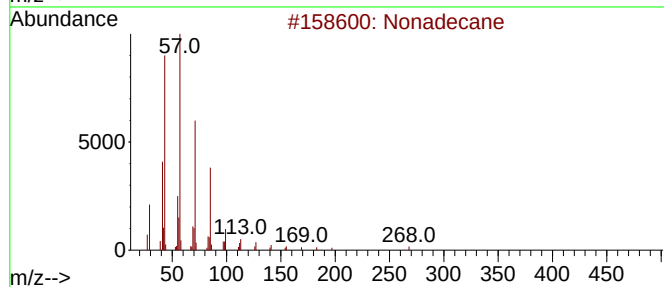
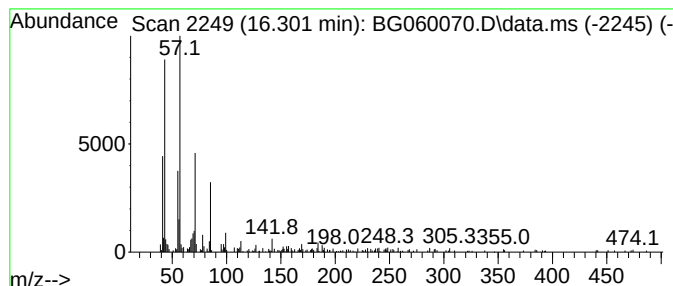
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Nonadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.301	3.99 ng	275278	Phenanthrene-d10	17.341

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Nonadecane	268	C19H40	000629-92-5	91
2		Docosane	310	C22H46	000629-97-0	83
3		Heptadecane	240	C17H36	000629-78-7	83
4		Tridecane	184	C13H28	000629-50-5	81
5		Pentadecane	212	C15H32	000629-62-9	76



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG121823\
Data File : BG060070.D
Acq On : 18 Dec 2023 17:33
Operator : MA/JU
Sample : 05796-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
RT-SB-06-12-13

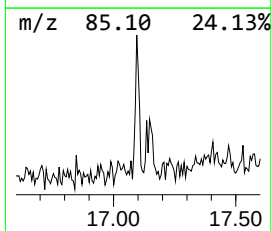
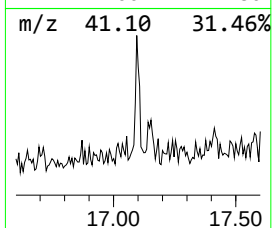
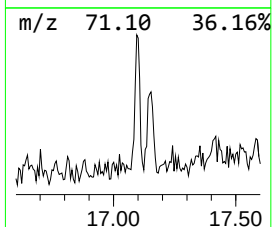
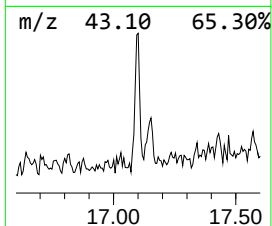
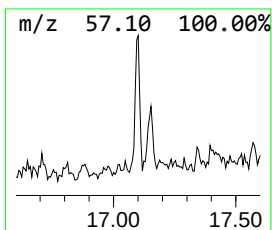
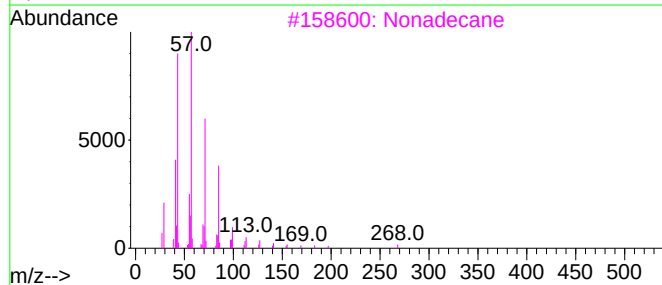
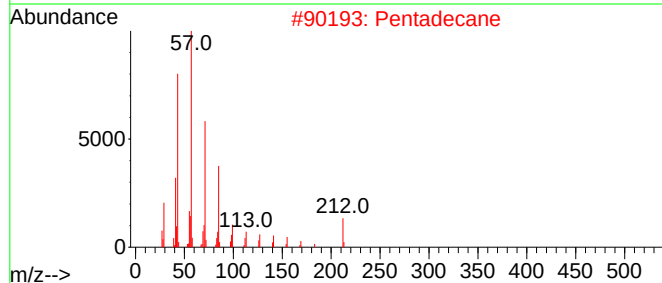
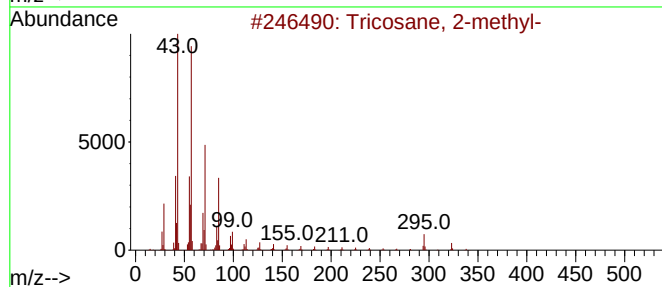
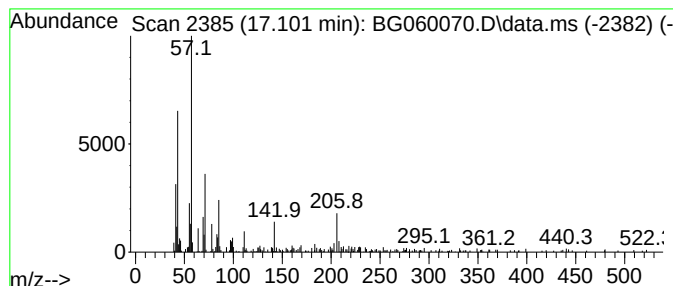
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Tricosane, 2-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.101	2.14 ng	147686	Phenanthrene-d10	17.341

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tricosane, 2-methyl-	338	C24H50	001928-30-9	50
2		Pentadecane	212	C15H32	000629-62-9	42
3		Nonadecane	268	C19H40	000629-92-5	42
4		Tetradecane, 2,6,10-trimethyl-	240	C17H36	014905-56-7	30
5		Dodecyl isobutyl ether	242	C16H34O	1000406-32-6	30



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG121823\
Data File : BG060070.D
Acq On : 18 Dec 2023 17:33
Operator : MA/JU
Sample : 05796-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

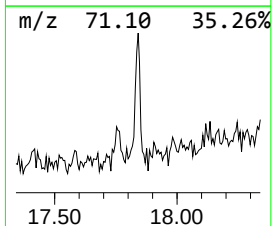
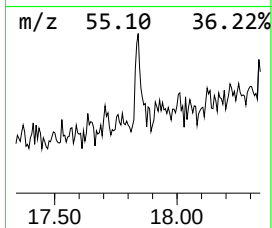
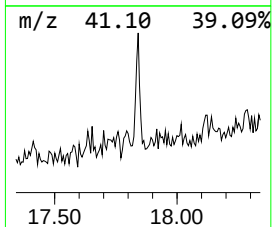
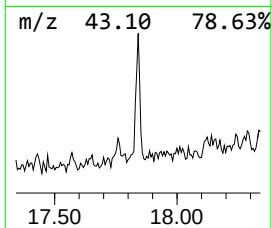
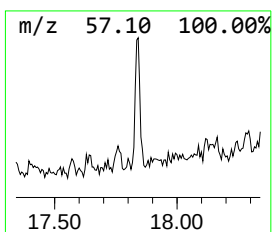
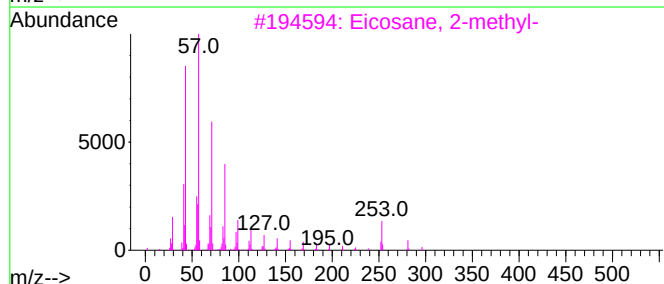
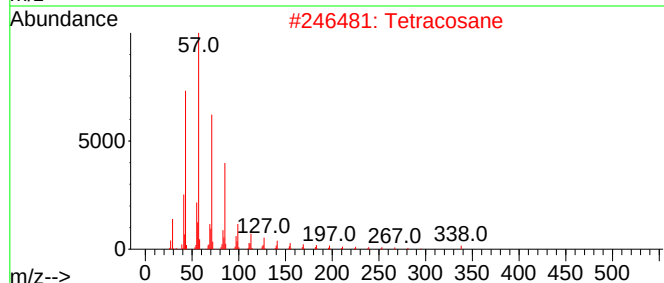
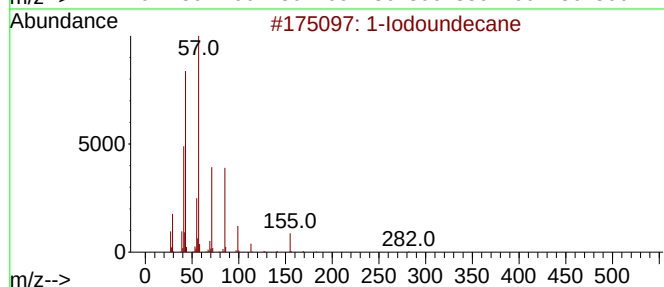
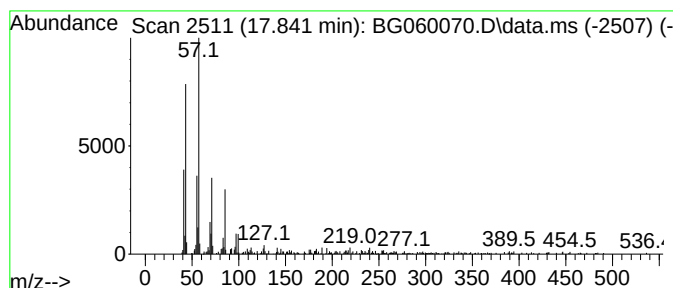
Instrument :
BNA_G
ClientSampleId :
RT-SB-06-12-13

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121323.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 1-Iodoundecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
17.841	3.31 ng	228487	Phenanthrene-d10	17.341	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Iodoundecane	282	C11H23I	004282-44-4	76
2	Tetracosane	338	C24H50	000646-31-1	70
3	Eicosane, 2-methyl-	296	C21H44	001560-84-5	68
4	Docosane, 7-hexyl-	394	C28H58	055373-86-9	68
5	Heptadecane	240	C17H36	000629-78-7	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG121823\
Data File : BG060070.D
Acq On : 18 Dec 2023 17:33
Operator : MA/JU
Sample : 05796-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
RT-SB-06-12-13

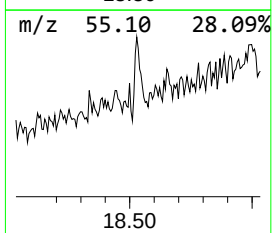
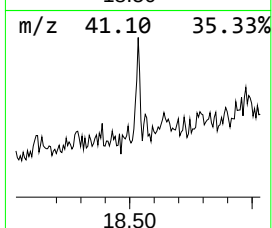
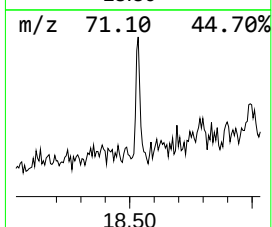
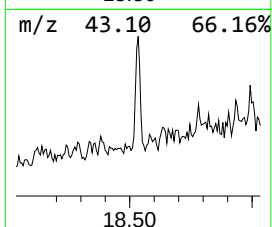
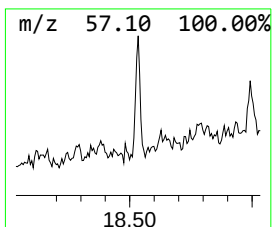
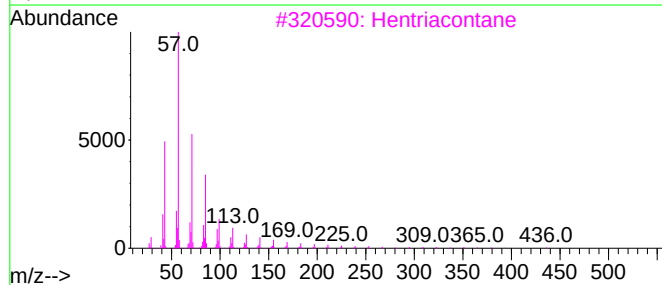
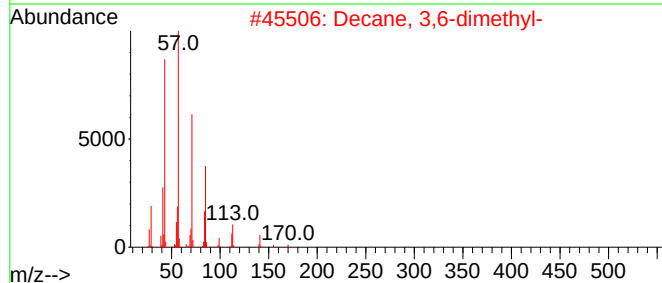
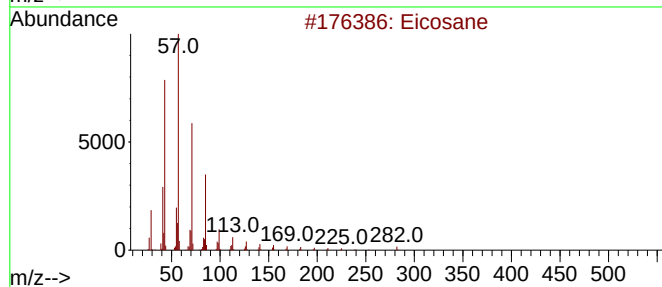
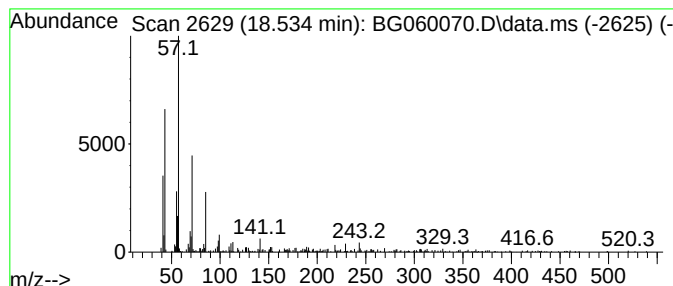
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Eicosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.534	4.09 ng	282168	Phenanthrene-d10	17.341

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eicosane	282	C20H42	000112-95-8	86
2			Decane, 3,6-dimethyl-	170	C12H26	017312-53-7	74
3			Hentriacontane	437	C31H64	000630-04-6	72
4			Decane, 3,8-dimethyl-	170	C12H26	017312-55-9	70
5			Decane, 2,6,8-trimethyl-	184	C13H28	062108-26-3	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG121823\
Data File : BG060070.D
Acq On : 18 Dec 2023 17:33
Operator : MA/JU
Sample : 05796-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

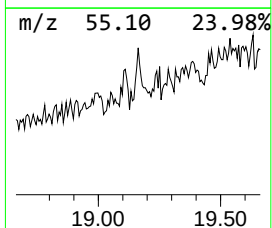
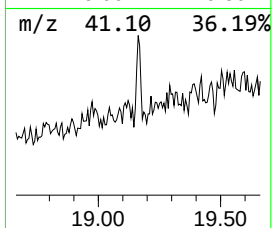
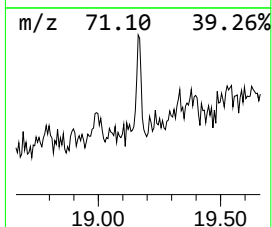
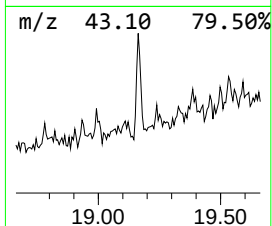
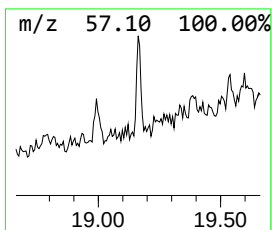
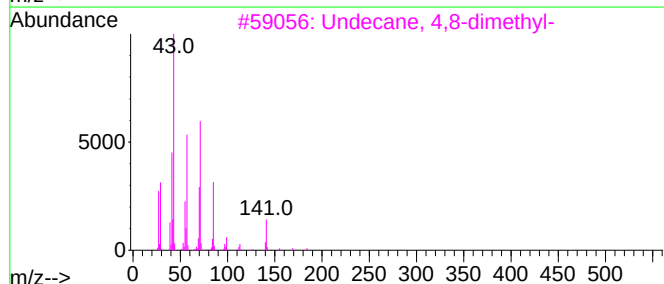
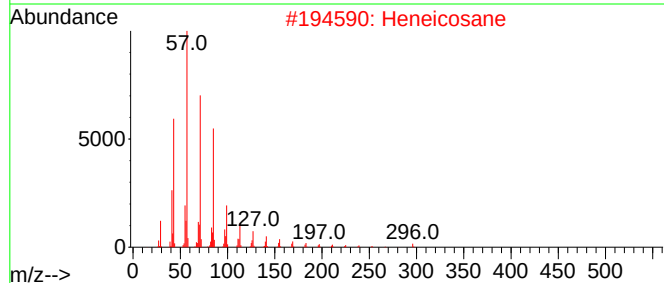
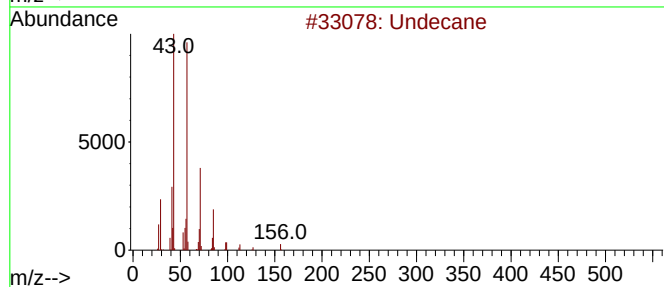
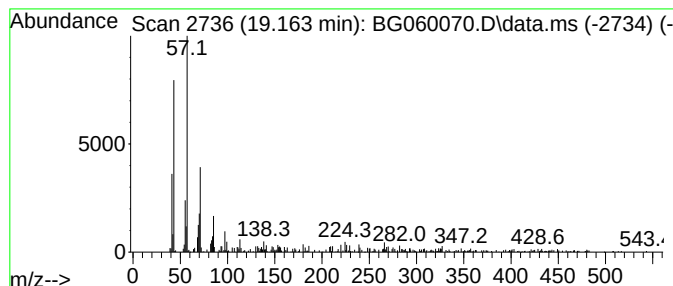
Instrument :
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ClientSampleId :
RT-SB-06-12-13

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121323.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Undecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.	
19.163	2.37 ng	163748	Phenanthrene-d10	17.341	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecane	156	C11H24	001120-21-4	60
2	Heneicosane	296	C21H44	000629-94-7	53
3	Undecane, 4,8-dimethyl-	184	C13H28	017301-33-6	49
4	Nonadecane	268	C19H40	000629-92-5	49
5	1-Heptene, 4-methyl-	112	C8H16	013151-05-8	49



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG121823\
Data File : BG060070.D
Acq On : 18 Dec 2023 17:33
Operator : MA/JU
Sample : 05796-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
RT-SB-06-12-13

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121323.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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3-Hexen-2-one	4.462	9.1	ng	207288	1	7.952	456582	20.0
2-Pentanone, 4-...	5.068	115.3	ng	2632250	1	7.952	456582	20.0
Dodecane, 2,6,1...	14.492	3.0	ng	154947	3	14.598	1038990	20.0
Heneicosane	15.438	2.3	ng	117762	3	14.598	1038990	20.0
Nonadecane	16.301	4.0	ng	275278	4	17.341	1381340	20.0
Tricosane, 2-me...	17.101	2.1	ng	147686	4	17.341	1381340	20.0
1-Iodoundecane	17.841	3.3	ng	228487	4	17.341	1381340	20.0
Eicosane	18.534	4.1	ng	282168	4	17.341	1381340	20.0
Undecane	19.163	2.4	ng	163748	4	17.341	1381340	20.0