

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG051724\
 Data File : BG061242.D
 Acq On : 17 May 2024 17:14
 Operator : MA/JU
 Sample : P2495-01
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 RT-3463

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-BG043024.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG061242.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.064	9	13	22	rBV7	9954	25312	1.62%	0.257%
2	3.153	22	28	44	rVB	255374	458089	29.24%	4.643%
3	3.675	112	117	125	rBV	15169	25603	1.63%	0.259%
4	5.526	426	432	446	rVB	419287	666894	42.57%	6.759%
5	7.113	695	702	714	rBV	437849	728294	46.49%	7.381%
6	7.929	835	841	848	rVB	114077	188216	12.01%	1.908%
7	9.087	1030	1038	1049	rBV	277051	483496	30.86%	4.900%
8	10.726	1310	1317	1324	rBV	149513	261395	16.69%	2.649%
9	13.182	1727	1735	1742	rBV	672452	1046566	66.80%	10.607%
10	14.557	1963	1969	1977	rVB	221060	347002	22.15%	3.517%
11	14.774	1998	2006	2012	rBV5	11878	27341	1.75%	0.277%
12	16.055	2217	2224	2232	rBV	516172	834218	53.25%	8.455%
13	17.307	2431	2437	2441	rBV	290975	423490	27.03%	4.292%
14	17.348	2441	2444	2449	rVB	55892	81536	5.20%	0.826%
15	18.229	2592	2594	2600	rVB2	20765	28708	1.83%	0.291%
16	18.376	2614	2619	2623	rBV3	22929	38617	2.46%	0.391%
17	18.417	2623	2626	2633	rVB2	13743	19795	1.26%	0.201%
18	18.581	2649	2654	2662	rBV8	14567	23097	1.47%	0.234%
19	18.681	2666	2671	2675	rBV	14498	21308	1.36%	0.216%
20	18.728	2675	2679	2686	rVB5	15289	22826	1.46%	0.231%
21	19.099	2738	2742	2745	rBV	17499	26028	1.66%	0.264%
22	19.240	2762	2766	2773	rBV6	11397	20224	1.29%	0.205%
23	19.363	2782	2787	2794	rBV	174307	242944	15.51%	2.462%
24	19.510	2809	2812	2817	rVB5	18989	24208	1.55%	0.245%
25	19.668	2836	2839	2840	rBV3	15150	17387	1.11%	0.176%
26	19.727	2840	2849	2857	rVB	167944	286911	18.31%	2.908%
27	19.798	2857	2861	2865	rBV7	14873	20718	1.32%	0.210%
28	19.927	2876	2883	2894	rBV	1167112	1566624	100.00%	15.877%
29	20.050	2899	2904	2910	rVV5	17754	39501	2.52%	0.400%
30	20.191	2923	2928	2930	rBV6	13921	27932	1.78%	0.283%
31	20.221	2930	2933	2941	rVB2	27908	50823	3.24%	0.515%
32	20.379	2957	2960	2964	rVB	20880	28211	1.80%	0.286%
33	20.520	2981	2984	2988	rBV	14976	19464	1.24%	0.197%
34	20.562	2988	2991	2995	rVB3	16355	23343	1.49%	0.237%
35	21.231	3101	3105	3112	rVB5	36687	76321	4.87%	0.773%
36	21.566	3155	3162	3167	rBV2	314194	612317	39.09%	6.206%

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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-BG043024.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	21.613	3167	3170	3175	rVB	94178	130417	8.32%	1.322%
38	23.705	3520	3526	3534	rBV2	51942	157290	10.04%	1.594%
39	24.404	3640	3645	3654	rVB	39203	97639	6.23%	0.990%
40	24.545	3663	3669	3678	rVB2	47550	122240	7.80%	1.239%
41	24.692	3686	3694	3706	rBV	181085	524782	33.50%	5.318%

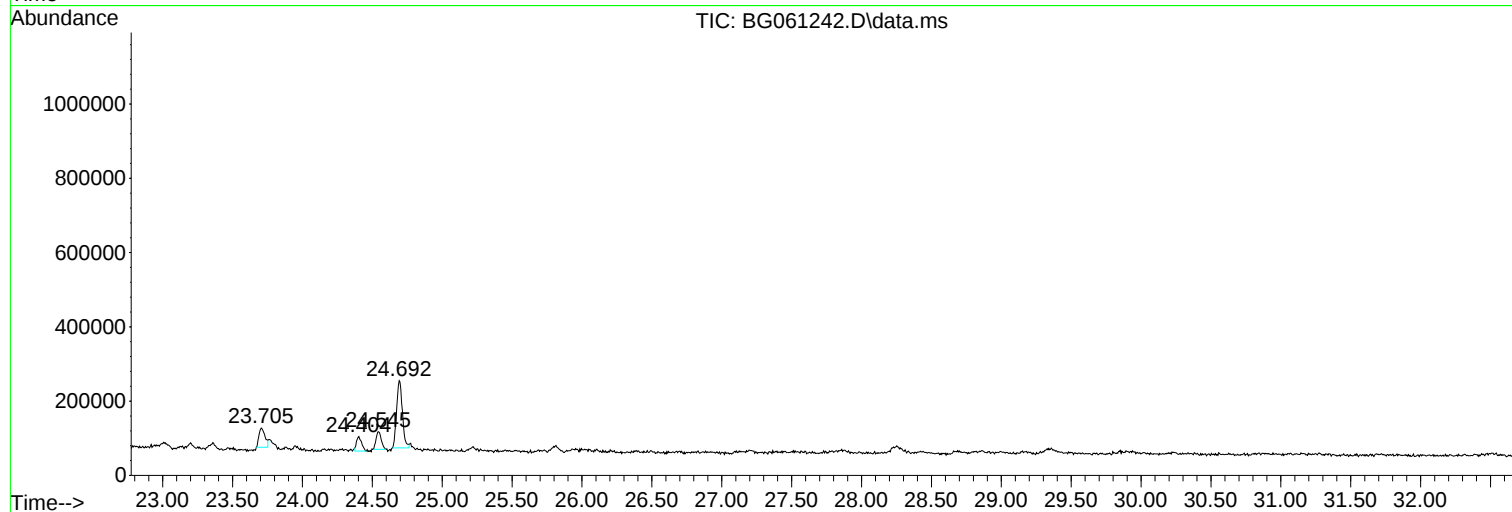
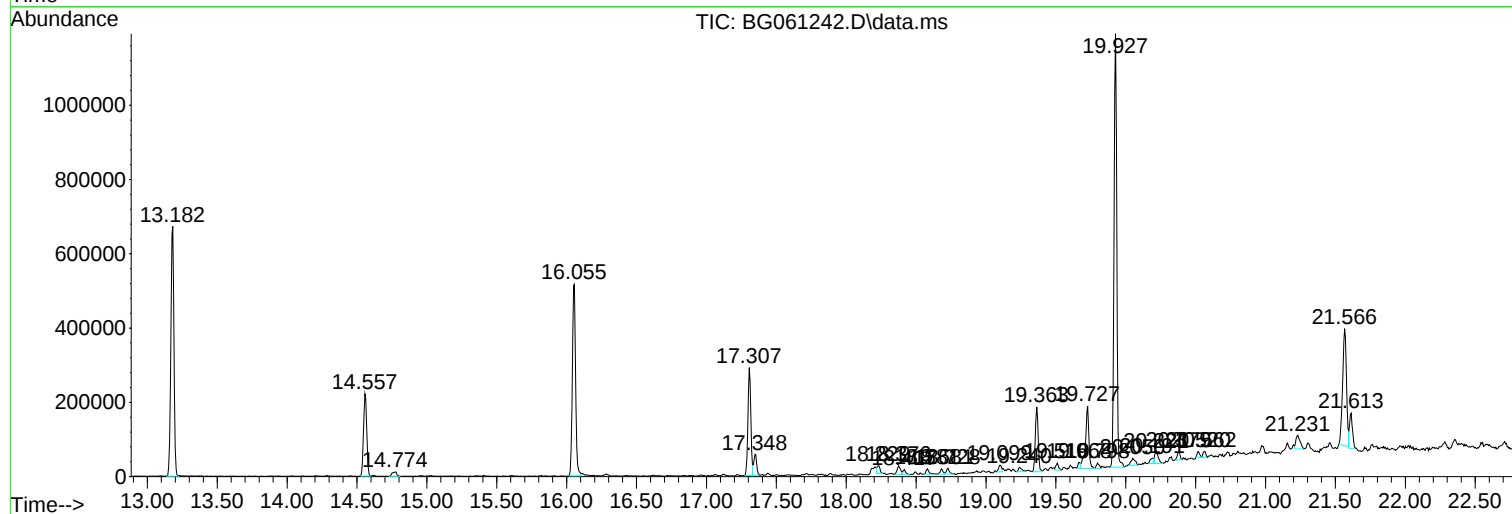
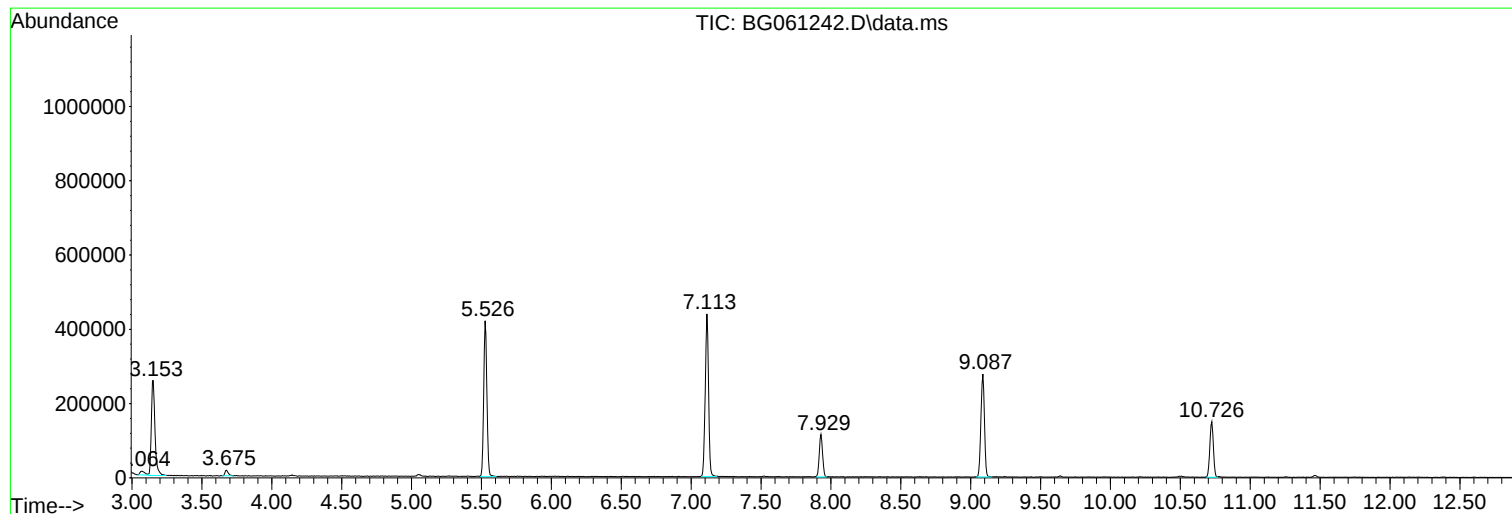
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG043024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Operator : MA/JU
Sample : P2495-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
RT-3463

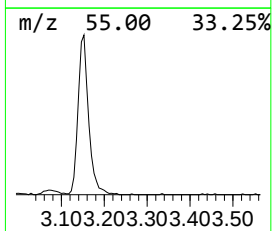
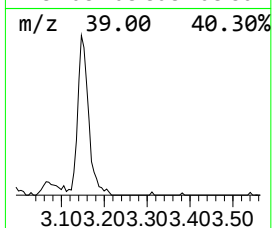
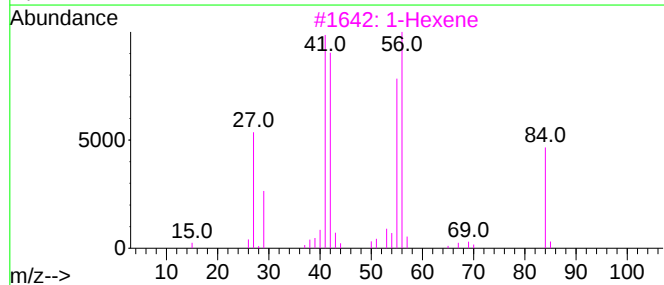
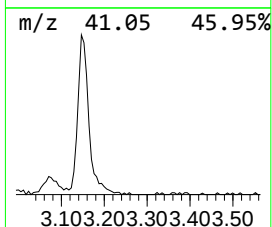
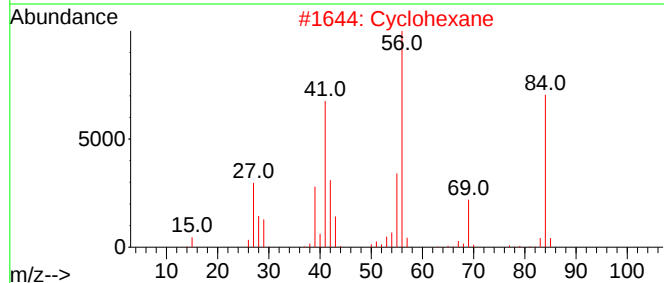
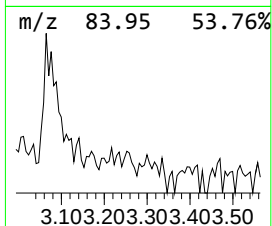
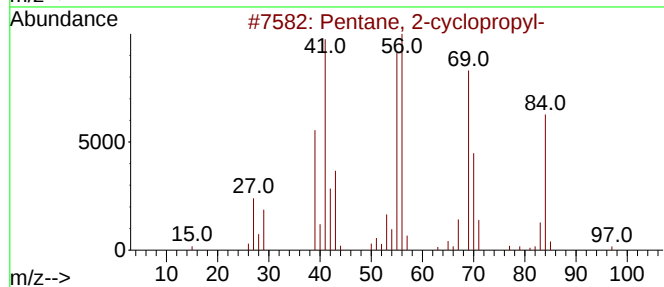
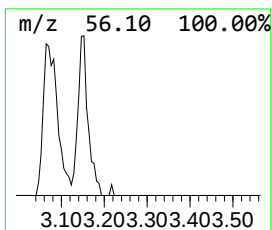
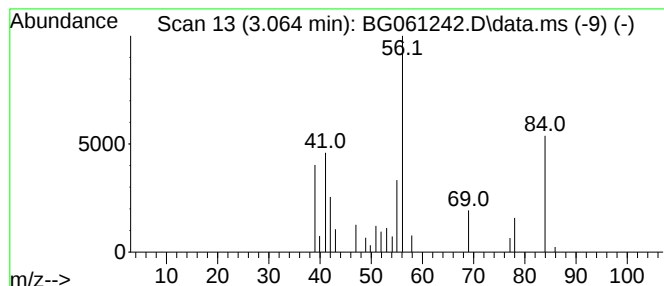
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG043024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Pentane, 2-cyclopropyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.064	2.69 ng	25312	1,4-Dichlorobenzene-d4	7.929

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2-cyclopropyl-	112	C8H16	005458-16-2	50
2			Cyclohexane	84	C6H12	000110-82-7	49
3			1-Hexene	84	C6H12	000592-41-6	37
4			Cyclobutanone, 2-methyl-	84	C5H8O	001517-15-3	23
5			Cyclobutane, ethyl-	84	C6H12	004806-61-5	17



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Sample : P2495-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
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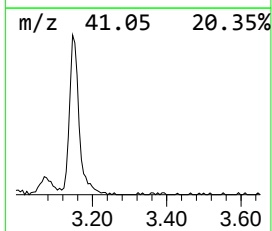
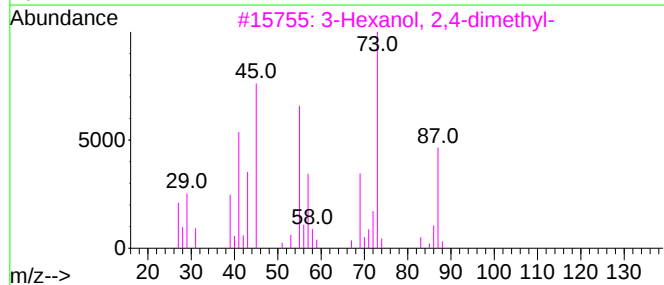
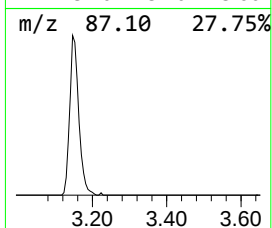
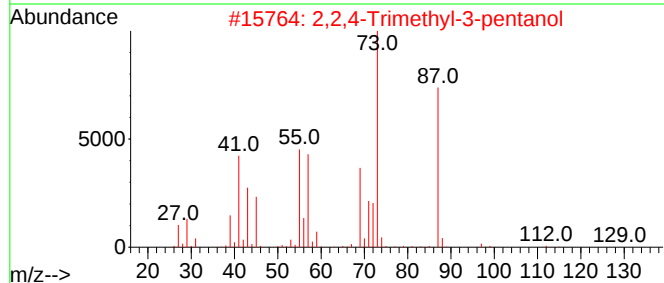
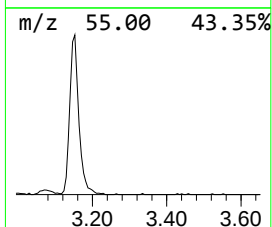
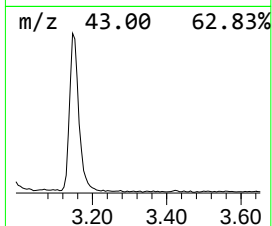
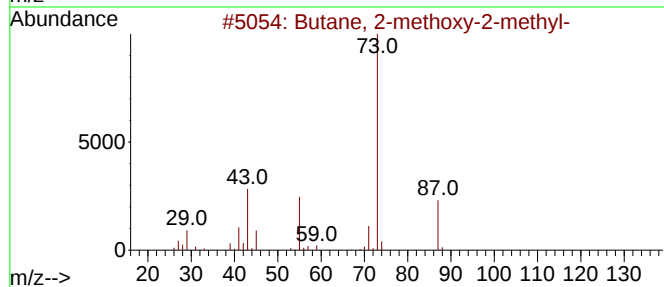
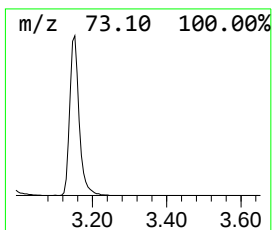
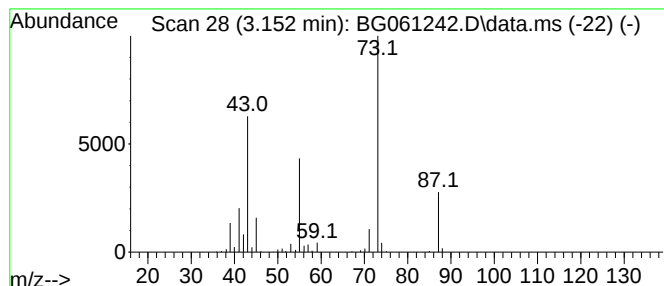
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG043024.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.152	48.68 ng	458089	1,4-Dichlorobenzene-d4	7.929

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	38
3			3-Hexanol, 2,4-dimethyl-	130	C8H18O	013432-25-2	33
4			3-Pentanol, 3-methyl-	102	C6H14O	000077-74-7	28
5			2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	12



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Misc :
ALS Vial : 12 Sample Multiplier: 1

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ClientSampleId :
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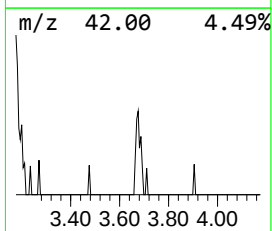
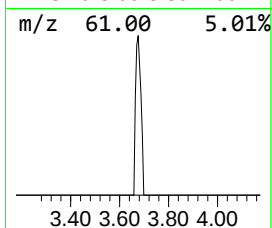
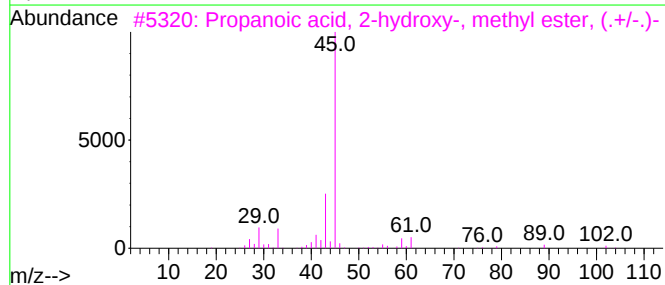
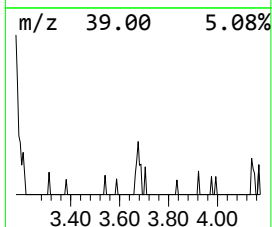
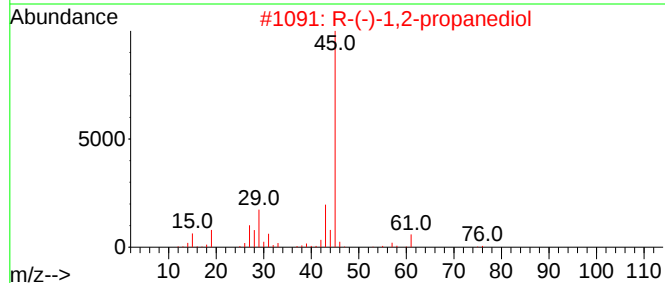
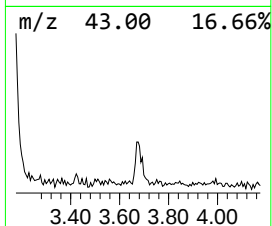
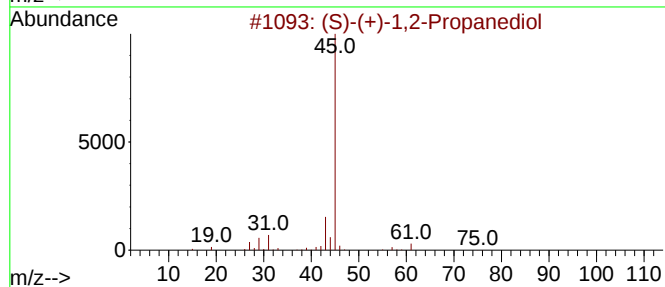
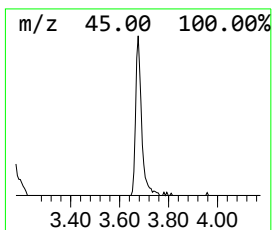
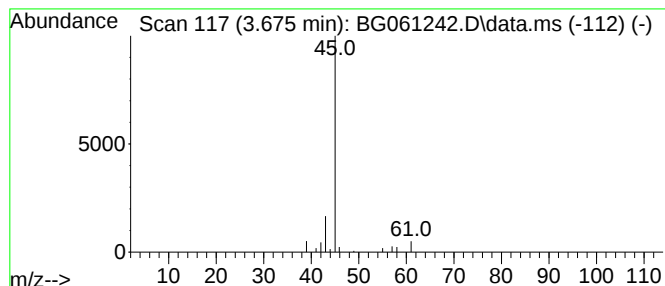
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG043024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 unknown3.675 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.675	2.72 ng	25603	1,4-Dichlorobenzene-d4	7.929

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	(S)-(+)-1,2-Propanediol			76	C3H8O2	004254-15-3	9
2	R-(-)-1,2-propanediol			76	C3H8O2	004254-14-2	9
3	Propanoic acid, 2-hydroxy-, meth...			104	C4H8O3	000547-64-8	9
4	Formamide			45	CH3NO	000075-12-7	7
5	2-Butanol, (R)-			74	C4H10O	014898-79-4	4



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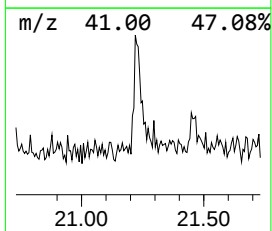
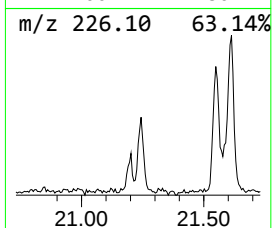
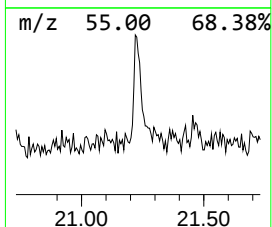
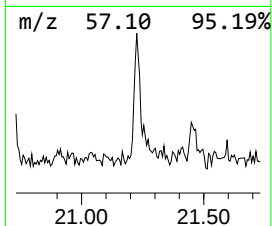
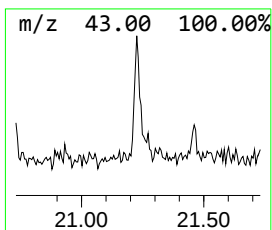
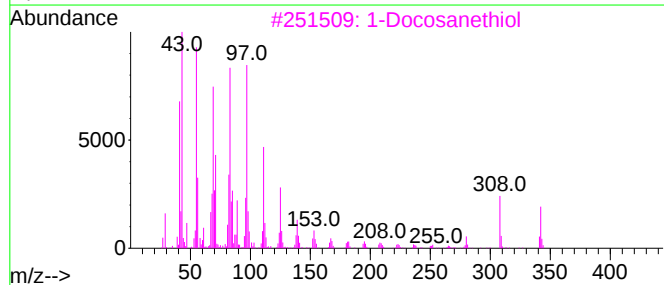
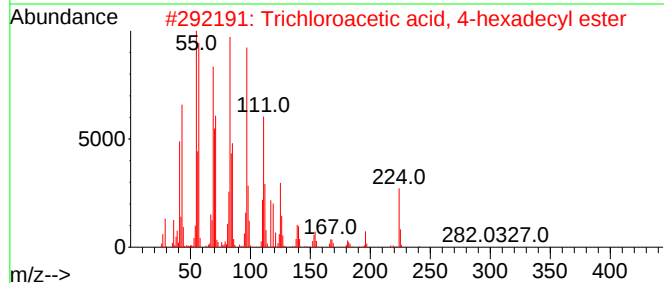
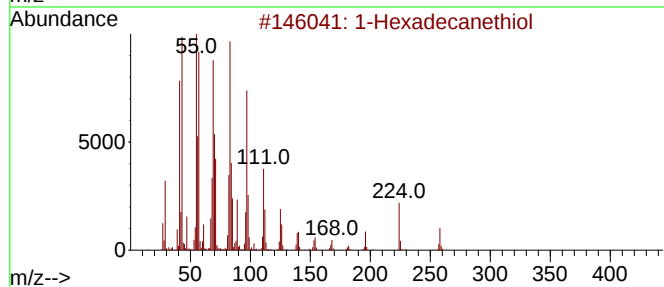
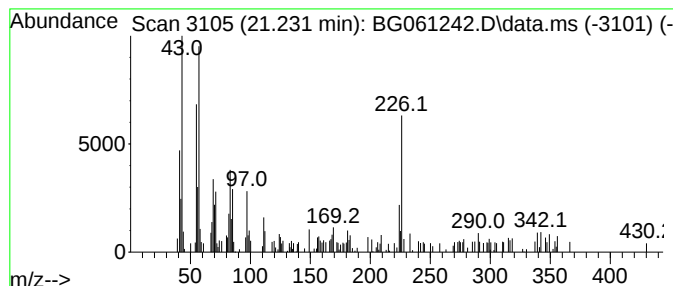
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 1-Hexadecanethiol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.231	2.49 ng	76321	Chrysene-d12	21.566

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexadecanethiol	258	C16H34S	002917-26-2	59
2			Trichloroacetic acid, 4-hexadecy...	386	C18H33Cl3O2	1000282-92-4	30
3			1-Docosanethiol	342	C22H46S	007773-83-3	25
4			Heptadecafluorononanoic acid, he...	688	C25H33F17O2	1000356-03-2	25
5			Octadecane, 1-(methylthio)-	300	C19H40S	040289-98-3	25



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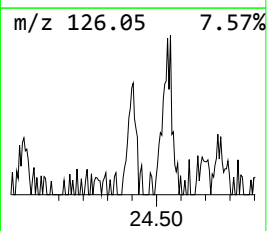
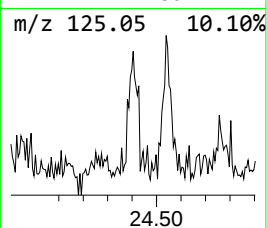
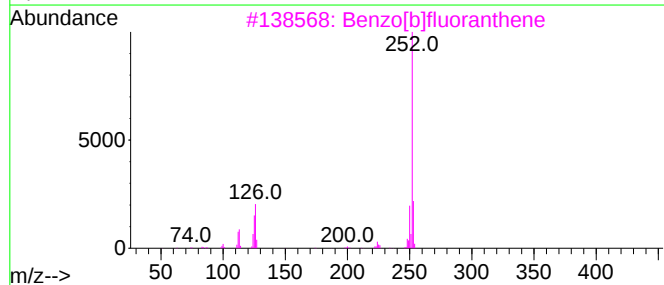
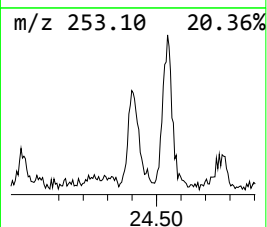
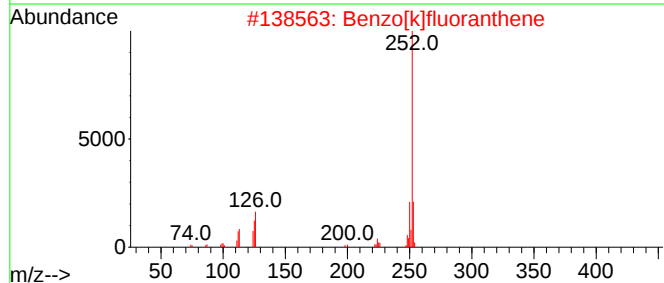
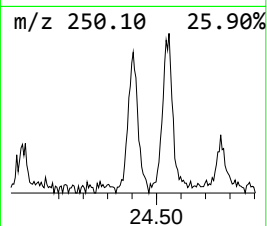
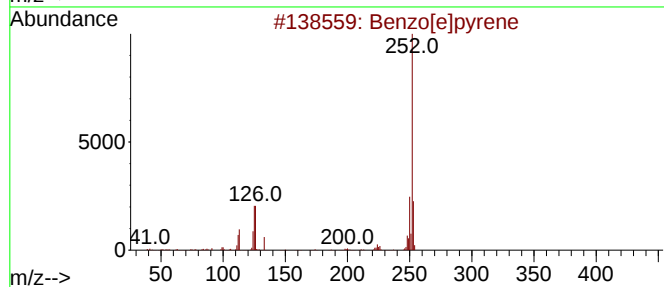
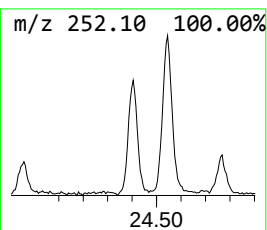
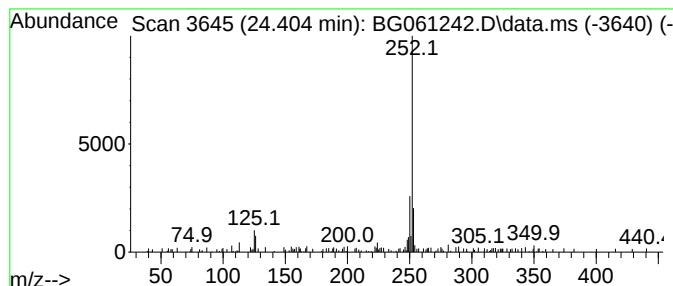
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG043024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Benzo[e]pyrene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.404	3.72 ng	97639	Perylene-d12	24.692

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[e]pyrene	252	C20H12	000192-97-2	76
2			Benzo[k]fluoranthene	252	C20H12	000207-08-9	76
3			Benzo[b]fluoranthene	252	C20H12	000205-99-2	76
4			(1-Cyclopentenyl)ferrocene	252	C15H16Fe	012260-67-2	72
5			Perylene	252	C20H12	000198-55-0	68



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG051724\
Data File : BG061242.D
Acq On : 17 May 2024 17:14
Operator : MA/JU
Sample : P2495-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
RT-3463

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG043024.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
Pentane, 2-cycl...	3.064	2.7	ng	25312	1	7.929	188216	20.0
Butane, 2-metho...	3.152	48.7	ng	458089	1	7.929	188216	20.0
unknown3.675	3.675	2.7	ng	25603	1	7.929	188216	20.0
1-Hexadecanethiol	21.231	2.5	ng	76321	5	21.566	612317	20.0
Benzo[e]pyrene	24.404	3.7	ng	97639	6	24.692	524782	20.0