

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG091422\
 Data File : BG054952.D
 Acq On : 14 Sep 2022 20:50
 Operator : CG/JU
 Sample : N4579-03 10X
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 CHERRY-HILL-COMP-11

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-BG082522.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG054952.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.285	333	340	346	rVB2	7324	12607	1.82%	0.247%
2	5.679	401	407	419	rVB	50444	87789	12.66%	1.717%
3	6.367	518	524	525	rBV2	5373	7341	1.06%	0.144%
4	6.760	585	591	603	rVB5	7330	18903	2.73%	0.370%
5	7.260	670	676	677	rBV2	15292	20678	2.98%	0.405%
6	7.295	677	682	696	rVB	49250	98554	14.21%	1.928%
7	8.053	799	811	813	rBV3	4388	10537	1.52%	0.206%
8	8.135	819	825	834	rVB	185948	316295	45.62%	6.188%
9	8.300	848	853	860	rVB7	4052	7262	1.05%	0.142%
10	8.693	915	920	925	rVB3	6961	13944	2.01%	0.273%
11	8.981	963	969	973	rBV8	7389	19681	2.84%	0.385%
12	9.234	1002	1012	1018	rBV5	10358	27872	4.02%	0.545%
13	9.316	1018	1026	1035	rBV	32801	75524	10.89%	1.477%
14	9.398	1035	1040	1044	rVB2	7432	11838	1.71%	0.232%
15	9.445	1044	1048	1051	rBV4	3993	7318	1.06%	0.143%
16	9.686	1082	1089	1093	rBV6	5502	14503	2.09%	0.284%
17	9.763	1098	1102	1107	rVB4	7395	11715	1.69%	0.229%
18	9.821	1107	1112	1115	rBV5	6472	9980	1.44%	0.195%
19	9.868	1115	1120	1131	rVB7	11413	26088	3.76%	0.510%
20	9.992	1131	1141	1143	rBV7	6093	14719	2.12%	0.288%
21	10.127	1158	1164	1170	rBV5	14579	28811	4.16%	0.564%
22	10.268	1183	1188	1195	rVB9	4835	11061	1.60%	0.216%
23	10.344	1196	1201	1207	rBV8	5518	12135	1.75%	0.237%
24	10.644	1245	1252	1259	rBV3	15283	40826	5.89%	0.799%
25	10.714	1259	1264	1269	rBV5	13327	28144	4.06%	0.551%
26	10.838	1280	1285	1291	rBV6	7842	14655	2.11%	0.287%
27	10.908	1291	1297	1300	rVV6	10611	23177	3.34%	0.453%
28	10.961	1300	1306	1318	rVV	245875	475552	68.59%	9.303%
29	11.085	1322	1327	1333	rVB	44299	74975	10.81%	1.467%
30	11.155	1334	1339	1345	rBV7	12136	27035	3.90%	0.529%
31	11.320	1359	1367	1370	rBV10	5345	14463	2.09%	0.283%
32	11.367	1373	1375	1380	rVV6	9017	15038	2.17%	0.294%
33	11.437	1381	1387	1392	rVB4	22725	44477	6.41%	0.870%
34	11.643	1414	1422	1429	rBV9	16937	40449	5.83%	0.791%
35	11.778	1439	1445	1448	rBV5	12709	26046	3.76%	0.510%
36	11.860	1454	1459	1465	rVB9	10979	28946	4.17%	0.566%

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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-BG082522.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	11.948	1467	1474	1478	rBV	41217	70971	10.24%	1.388%
38	11.995	1478	1482	1486	rVV4	25926	38378	5.54%	0.751%
39	12.136	1502	1506	1511	rBV4	15028	23996	3.46%	0.469%
40	12.224	1514	1521	1533	rVV4	19660	63597	9.17%	1.244%
41	12.559	1575	1578	1585	rVB5	33816	55638	8.02%	1.088%
42	12.689	1596	1600	1605	rVB4	17855	30873	4.45%	0.604%
43	12.747	1606	1610	1612	rBV5	9815	15222	2.20%	0.298%
44	12.971	1643	1648	1652	rBV6	22042	45569	6.57%	0.891%
45	13.282	1696	1701	1707	rBV2	55948	85994	12.40%	1.682%
46	13.394	1715	1720	1731	rVB	96016	160965	23.22%	3.149%
47	13.576	1743	1751	1758	rBV6	19469	54181	7.81%	1.060%
48	13.652	1760	1764	1768	rBV6	11865	22784	3.29%	0.446%
49	13.958	1813	1816	1820	rVB6	10779	13258	1.91%	0.259%
50	14.087	1835	1838	1842	rBV5	13588	19959	2.88%	0.390%
51	14.193	1851	1856	1858	rBV3	29382	48880	7.05%	0.956%
52	14.222	1858	1861	1865	rVB2	37980	52396	7.56%	1.025%
53	14.510	1905	1910	1915	rVB6	15619	28758	4.15%	0.563%
54	14.592	1921	1924	1929	rVB4	27053	38834	5.60%	0.760%
55	14.774	1949	1955	1963	rVB	384281	613054	88.42%	11.993%
56	14.974	1985	1989	1997	rVB9	12204	30148	4.35%	0.590%
57	15.380	2053	2058	2064	rBV2	18522	38164	5.50%	0.747%
58	15.550	2081	2087	2092	rBV9	13243	28838	4.16%	0.564%
59	16.261	2203	2208	2215	rBV	51968	90687	13.08%	1.774%
60	16.467	2238	2243	2250	rVB3	21520	38023	5.48%	0.744%
61	16.619	2265	2269	2273	rBV5	8393	13068	1.88%	0.256%
62	16.872	2310	2312	2315	rBV4	6269	7241	1.04%	0.142%
63	17.289	2379	2383	2387	rBV2	13216	18539	2.67%	0.363%
64	17.518	2416	2422	2428	rBV	428924	674714	97.31%	13.199%
65	18.394	2569	2571	2576	rBV3	7989	12036	1.74%	0.235%
66	19.304	2723	2726	2731	rBV	24432	36428	5.25%	0.713%
67	19.610	2775	2778	2784	rVB4	27000	39510	5.70%	0.773%
68	20.115	2860	2864	2869	rBV	149251	188706	27.22%	3.692%
69	21.813	3148	3153	3162	rVB	393967	693343	100.00%	13.564%

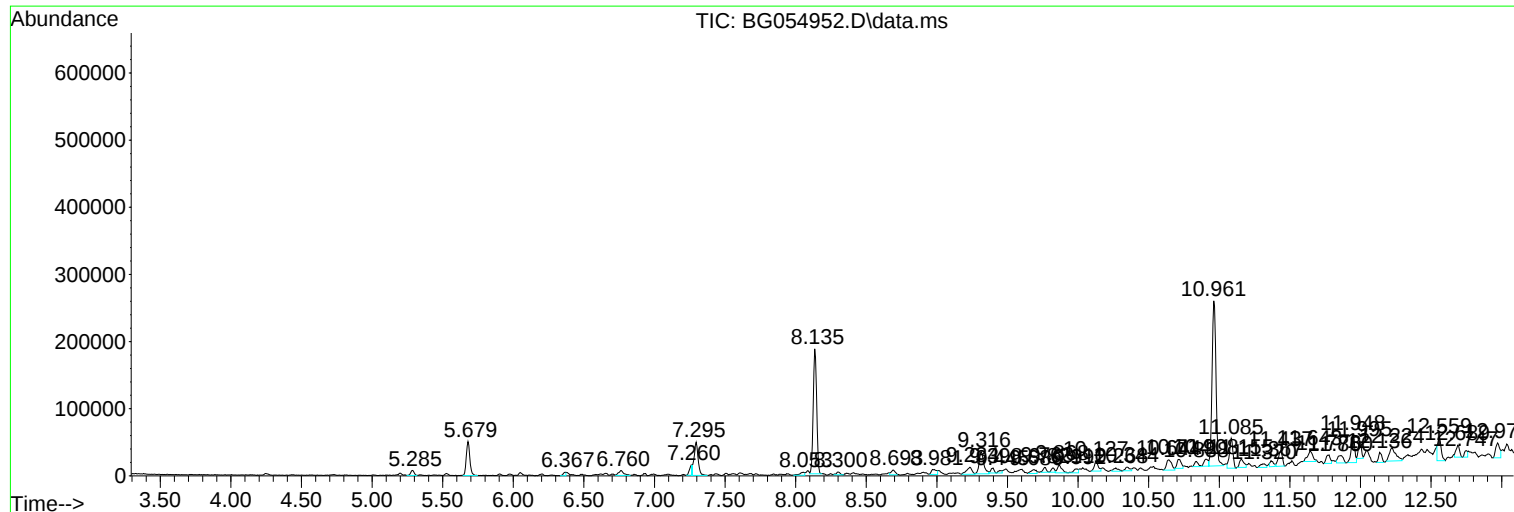
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ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
CHERRY-HILL-COMP-11

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG082522.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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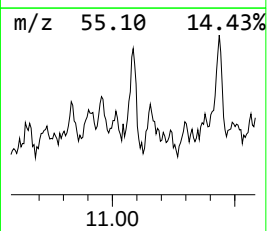
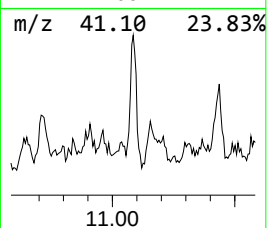
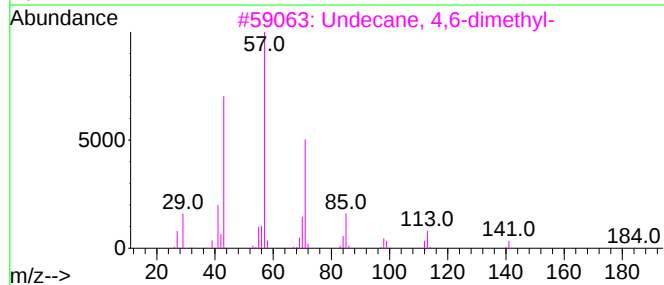
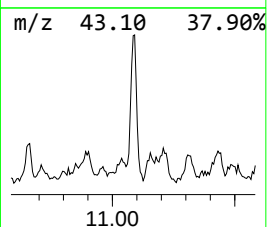
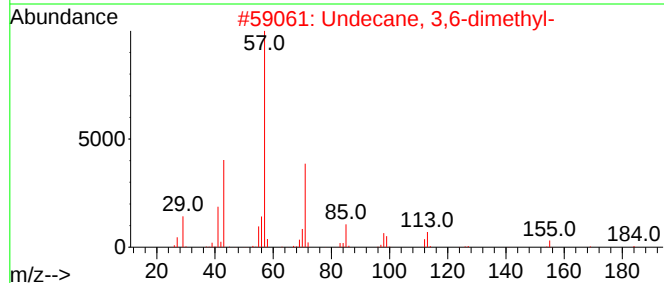
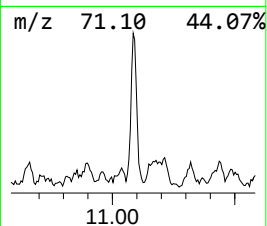
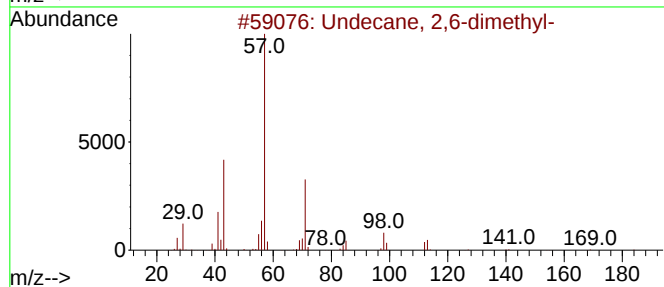
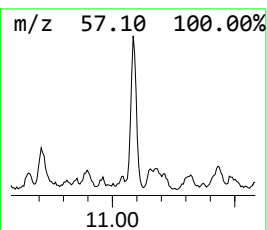
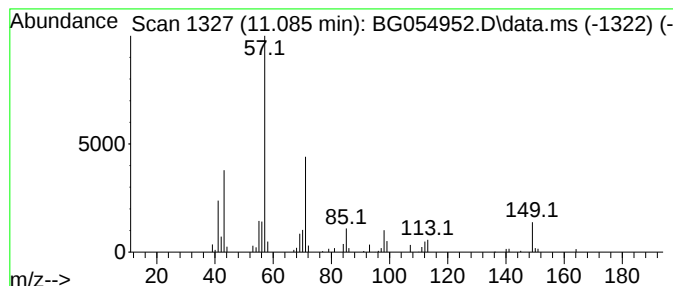
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG082522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Undecane, 2,6-dimethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.085	3.15 ng	74975	Naphthalene-d8	10.961

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Undecane, 2,6-dimethyl-	184	C13H28	017301-23-4	80
2			Undecane, 3,6-dimethyl-	184	C13H28	017301-28-9	78
3			Undecane, 4,6-dimethyl-	184	C13H28	017312-82-2	64
4			Hexadecane, 7-methyl-	240	C17H36	026730-20-1	64
5			Sulfurous acid, decyl 2-ethylhex...	334	C18H38O3S	1000309-19-3	64



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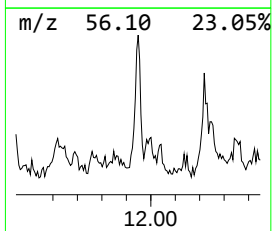
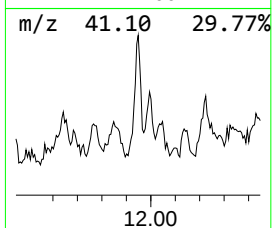
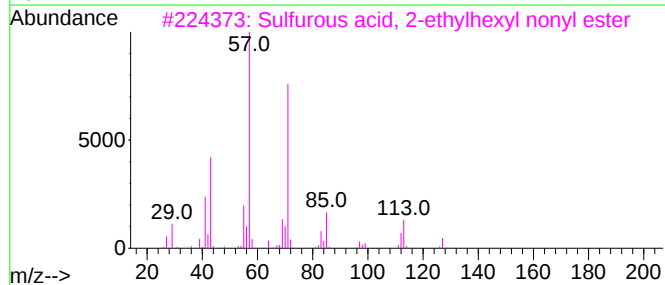
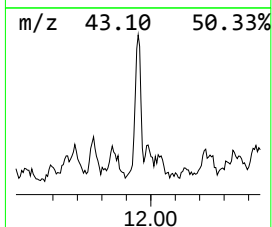
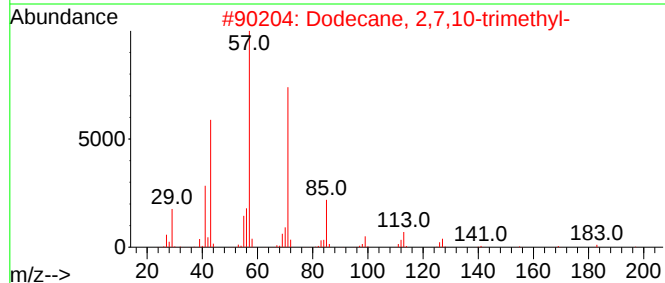
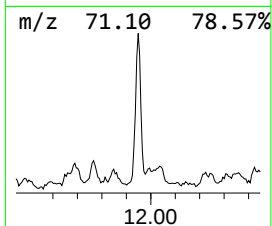
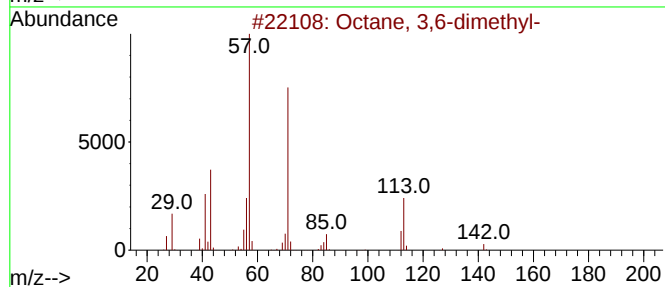
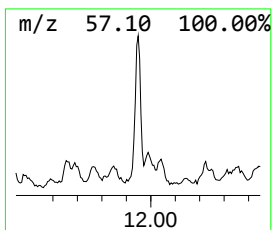
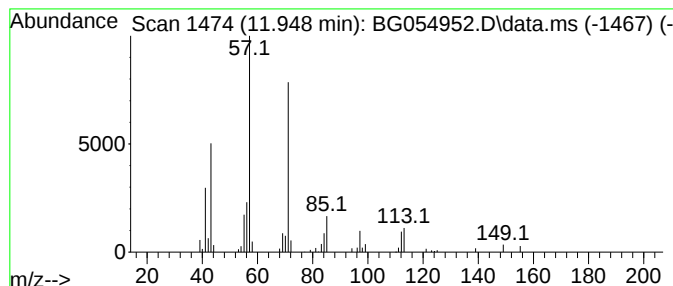
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG082522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Octane, 3,6-dimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.948	2.98 ng	70971	Naphthalene-d8	10.961

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octane, 3,6-dimethyl-	142	C10H22	015869-94-0	64
2			Dodecane, 2,7,10-trimethyl-	212	C15H32	074645-98-0	64
3			Sulfurous acid, 2-ethylhexyl non...	320	C17H36O3S	1010309-19-2	64
4			Octane, 1,1'-oxybis-	242	C16H34O	000629-82-3	64
5			6-Methyl-2-heptanol, 2-methylpro...	200	C12H24O2	1000447-36-7	59



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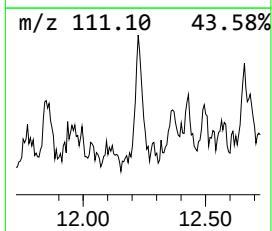
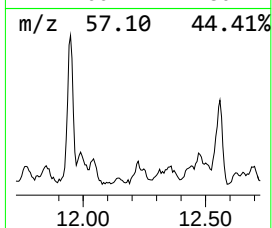
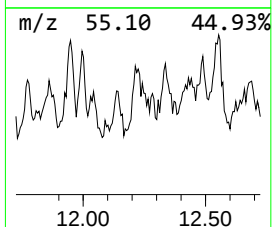
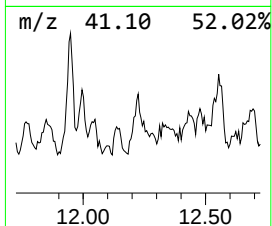
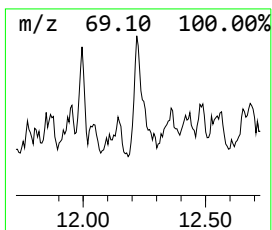
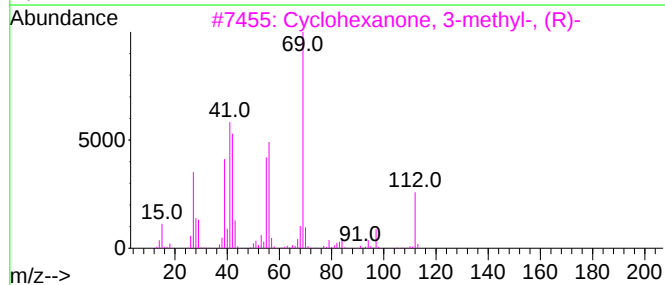
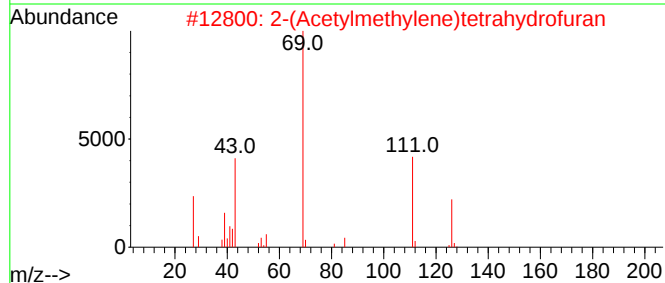
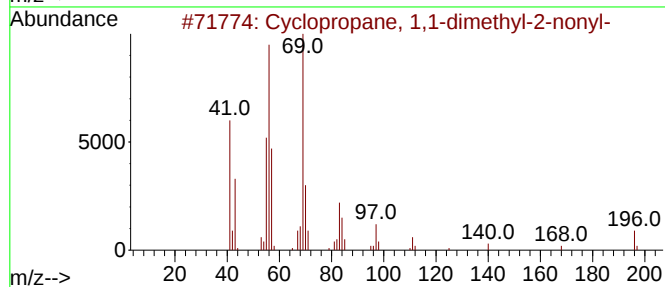
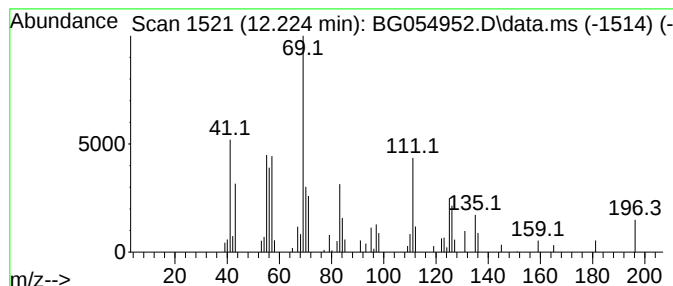
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown12.224 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.224	2.67 ng	63597	Naphthalene-d8	10.961

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopropane, 1,1-dimethyl-2-nonyl-	196	C14H28	041977-38-2	46
2			2-(Acetylmethylene)tetrahydrofuran	126	C7H10O2	112595-65-0	46
3			Cyclohexanone, 3-methyl-, (R)-	112	C7H12O	013368-65-5	43
4			Cyclohexanone, 3-methyl-	112	C7H12O	000591-24-2	43
5			3,4-Dimethyl cyclohexanone	126	C8H14O	005465-09-8	38



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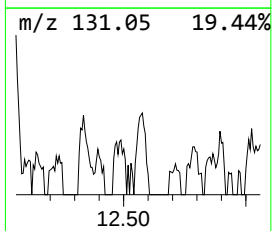
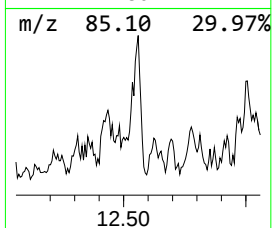
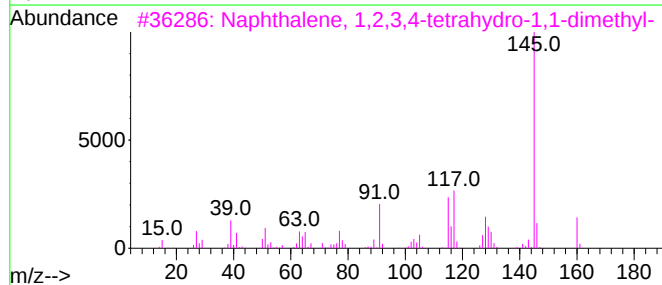
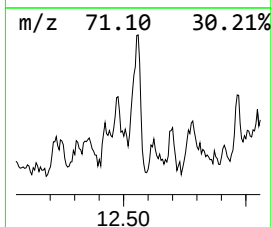
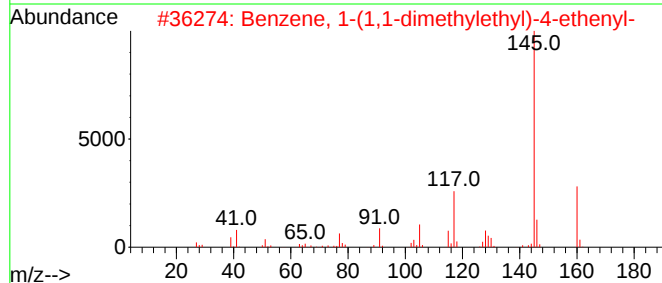
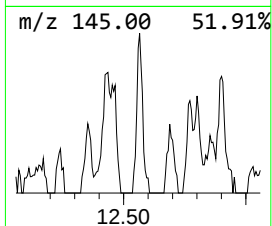
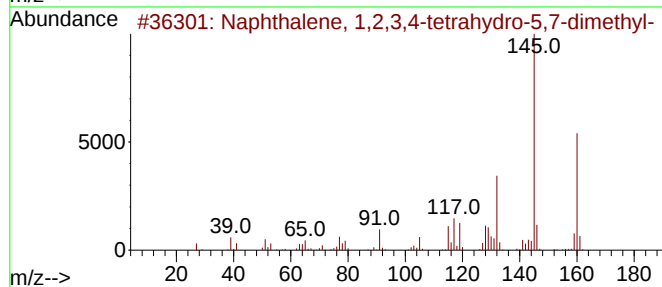
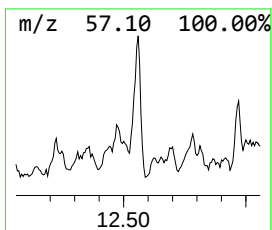
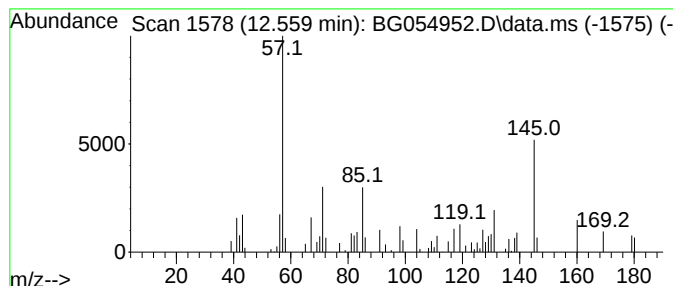
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG082522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 unknown12.559 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.559	2.34 ng	55638	Naphthalene-d8	10.961

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	021693-54-9	35
2			Benzene, 1-(1,1-dimethylethyl)-4...	160	C12H16	001746-23-2	27
3			Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	001985-59-7	27
4			1H-Indene, 2,3-dihydro-1,1,3-tri...	160	C12H16	002613-76-5	27
5			Benzene, 1-(1-methylethenyl)-3-(...	160	C12H16	001129-29-9	27



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG091422\
Data File : BG054952.D
Acq On : 14 Sep 2022 20:50
Operator : CG/JU
Sample : N4579-03 10X
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
CHERRY-HILL-COMP-11

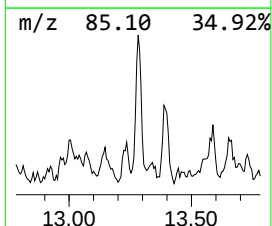
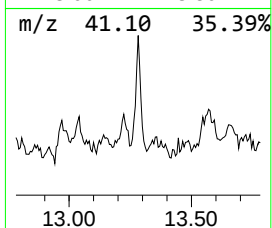
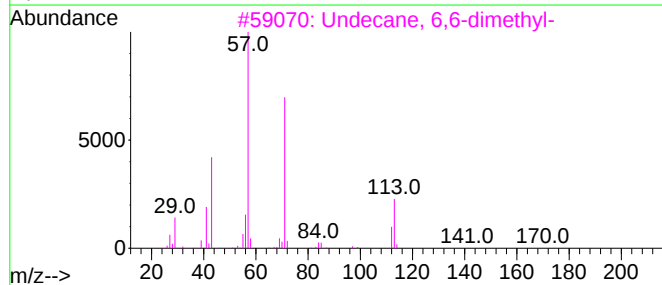
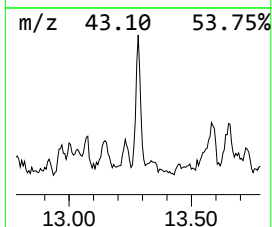
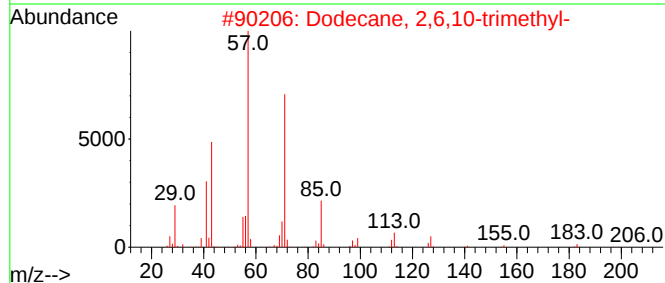
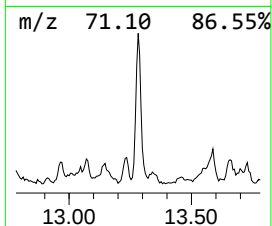
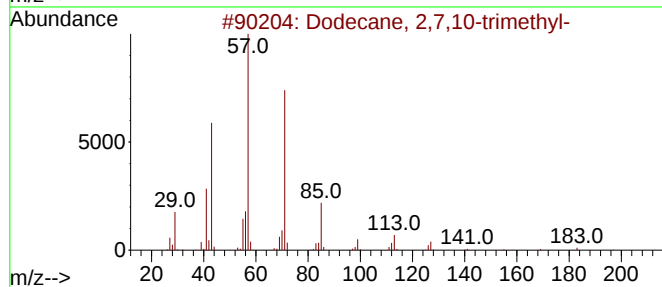
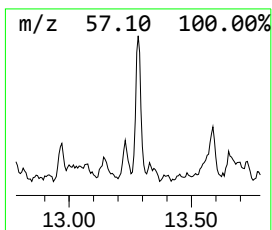
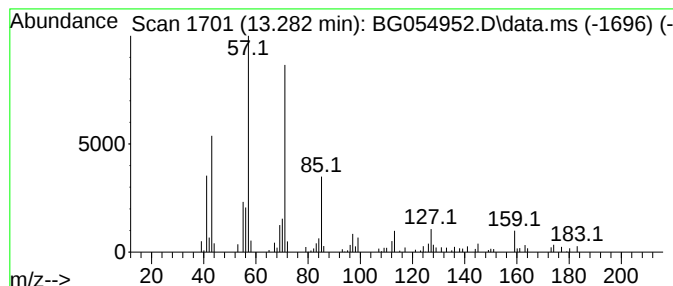
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Dodecane, 2,7,10-trimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.282	2.81 ng	85994	Acenaphthene-d10	14.774

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecane, 2,7,10-trimethyl-	212	C15H32	074645-98-0	72
2			Dodecane, 2,6,10-trimethyl-	212	C15H32	003891-98-3	64
3			Undecane, 6,6-dimethyl-	184	C13H28	017312-76-4	53
4			Nonane, 5-butyl-	184	C13H28	017312-63-9	47
5			Dodecane, 4,6-dimethyl-	198	C14H30	061141-72-8	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG091422\
Data File : BG054952.D
Acq On : 14 Sep 2022 20:50
Operator : CG/JU
Sample : N4579-03 10X
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
CHERRY-HILL-COMP-11

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG082522.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
Undecane, 2,6-d...	11.085	3.1	ng	74975	2	10.961	475552	20.0
Octane, 3,6-dim...	11.948	3.0	ng	70971	2	10.961	475552	20.0
unknown12.224	12.224	2.7	ng	63597	2	10.961	475552	20.0
unknown12.559	12.559	2.3	ng	55638	2	10.961	475552	20.0
Dodecane, 2,7,1...	13.282	2.8	ng	85994	3	14.774	613054	20.0