

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG091422\
 Data File : BG054950.D
 Acq On : 14 Sep 2022 19:27
 Operator : CG/JU
 Sample : N4579-19 5X
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 CHERRY-HILL-COMP-15

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: BG054950.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.200	318	325	331	rBV	5314	8737	1.19%	0.142%
2	5.676	400	406	416	rBV	93116	160245	21.76%	2.602%
3	7.291	667	681	692	rBV	92593	178820	24.29%	2.904%
4	8.084	811	816	818	rBV2	5788	8252	1.12%	0.134%
5	8.137	818	825	836	rVB	179518	318394	43.24%	5.170%
6	8.690	914	919	924	rVB3	4343	8998	1.22%	0.146%
7	9.236	1007	1012	1017	rVB5	5835	10616	1.44%	0.172%
8	9.312	1017	1025	1035	rVB	59211	119999	16.30%	1.948%
9	9.589	1069	1072	1078	rVB5	4896	10042	1.36%	0.163%
10	9.683	1080	1088	1094	rBV7	2849	9133	1.24%	0.148%
11	9.765	1097	1102	1106	rBV4	7997	12094	1.64%	0.196%
12	9.865	1115	1119	1129	rVB6	6315	14299	1.94%	0.232%
13	9.988	1134	1140	1142	rBV6	3963	7389	1.00%	0.120%
14	10.059	1147	1152	1156	rVV4	5298	9169	1.25%	0.149%
15	10.129	1156	1164	1169	rVV7	7245	13046	1.77%	0.212%
16	10.182	1169	1173	1181	rVB3	5901	14365	1.95%	0.233%
17	10.258	1181	1186	1189	rBV5	4228	7610	1.03%	0.124%
18	10.347	1196	1201	1207	rBV6	7152	13828	1.88%	0.225%
19	10.523	1225	1231	1238	rVB7	5008	12200	1.66%	0.198%
20	10.646	1246	1252	1258	rBV6	8233	20004	2.72%	0.325%
21	10.711	1258	1263	1272	rVV	32968	63043	8.56%	1.024%
22	10.905	1290	1296	1298	rBV2	12092	21419	2.91%	0.348%
23	10.963	1299	1306	1318	rVV	238994	457254	62.10%	7.425%
24	11.087	1321	1327	1332	rVB	30222	54164	7.36%	0.879%
25	11.157	1334	1339	1345	rBV5	7782	14973	2.03%	0.243%
26	11.363	1370	1374	1380	rBV6	3996	8297	1.13%	0.135%
27	11.433	1380	1386	1391	rVB6	12118	24123	3.28%	0.392%
28	11.639	1412	1421	1428	rBV10	12866	33486	4.55%	0.544%
29	11.768	1438	1443	1447	rBV5	7082	12694	1.72%	0.206%
30	11.845	1451	1456	1464	rVB8	8709	22718	3.09%	0.369%
31	11.945	1466	1473	1478	rBV	36981	61907	8.41%	1.005%
32	11.998	1478	1482	1486	rVV4	11819	20753	2.82%	0.337%
33	12.050	1486	1491	1495	rVB6	6510	12184	1.65%	0.198%
34	12.139	1502	1506	1510	rVB5	8330	12534	1.70%	0.204%
35	12.221	1512	1520	1527	rBV6	11593	33095	4.49%	0.537%
36	12.338	1533	1540	1544	rBV6	10481	20101	2.73%	0.326%

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

37	12.473	1558	1563	1570	rVV8	5544	15156	2.06%	0.246%
38	12.556	1570	1577	1584	rVB4	16853	39458	5.36%	0.641%
39	12.750	1605	1610	1614	rBV6	5409	12459	1.69%	0.202%
40	12.967	1642	1647	1650	rBV5	12138	21313	2.89%	0.346%
41	13.143	1674	1677	1683	rVB5	10104	17453	2.37%	0.283%
42	13.220	1684	1690	1695	rVV3	12532	26837	3.64%	0.436%
43	13.284	1695	1701	1710	rVV	45234	75246	10.22%	1.222%
44	13.390	1713	1719	1730	rVB	181674	293341	39.84%	4.763%
45	13.555	1742	1747	1749	rBV4	11364	19436	2.64%	0.316%
46	13.643	1758	1762	1769	rBV3	24424	41685	5.66%	0.677%
47	13.954	1813	1815	1820	rVB6	8603	11995	1.63%	0.195%
48	14.089	1833	1838	1843	rBV6	12643	24616	3.34%	0.400%
49	14.136	1843	1846	1850	rVV4	9467	12281	1.67%	0.199%
50	14.189	1850	1855	1857	rVV2	23392	35853	4.87%	0.582%
51	14.218	1857	1860	1864	rVB3	38085	51600	7.01%	0.838%
52	14.336	1877	1880	1885	rVB4	8793	11168	1.52%	0.181%
53	14.500	1904	1908	1914	rBV5	11683	24275	3.30%	0.394%
54	14.594	1918	1924	1930	rVB4	17035	28530	3.87%	0.463%
55	14.771	1940	1954	1962	rBV	376532	628010	85.30%	10.197%
56	14.976	1983	1989	1997	rBV	7765	17847	2.42%	0.290%
57	15.076	1998	2006	2007	rBV8	6588	12698	1.72%	0.206%
58	15.135	2012	2016	2019	rBV3	5650	8377	1.14%	0.136%
59	15.241	2030	2034	2044	rVB7	9532	23885	3.24%	0.388%
60	15.382	2053	2058	2061	rBV5	8394	15396	2.09%	0.250%
61	15.476	2071	2074	2078	rVB5	6925	10487	1.42%	0.170%
62	15.546	2080	2086	2091	rBV7	9794	20783	2.82%	0.337%
63	15.846	2135	2137	2145	rVB6	4051	7691	1.04%	0.125%
64	15.981	2154	2160	2165	rBV	17775	29629	4.02%	0.481%
65	16.257	2202	2207	2217	rBV	90269	152495	20.71%	2.476%
66	16.463	2235	2242	2247	rBV2	31544	56235	7.64%	0.913%
67	17.285	2378	2382	2387	rBV2	11068	14449	1.96%	0.235%
68	17.520	2413	2422	2435	rBV	434118	680525	92.43%	11.050%
69	18.155	2527	2530	2534	rVB2	9948	11770	1.60%	0.191%
70	18.578	2598	2602	2606	rBV6	4758	9050	1.23%	0.147%
71	18.684	2616	2620	2624	rBV6	6180	12122	1.65%	0.197%
72	18.790	2634	2638	2643	rVB8	5053	7803	1.06%	0.127%
73	19.107	2690	2692	2700	rVB8	6018	11920	1.62%	0.194%
74	19.318	2722	2728	2731	rBV4	23995	41563	5.65%	0.675%
75	19.448	2747	2750	2754	rBV4	11512	16604	2.26%	0.270%
76	20.117	2859	2864	2869	rBV	289477	367119	49.86%	5.961%

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

77	21.815	3147	3153	3160	rVB	395181	673222	91.44%	10.931%
78	25.194	3721	3728	3740	rVB2	239143	736272	100.00%	11.955%

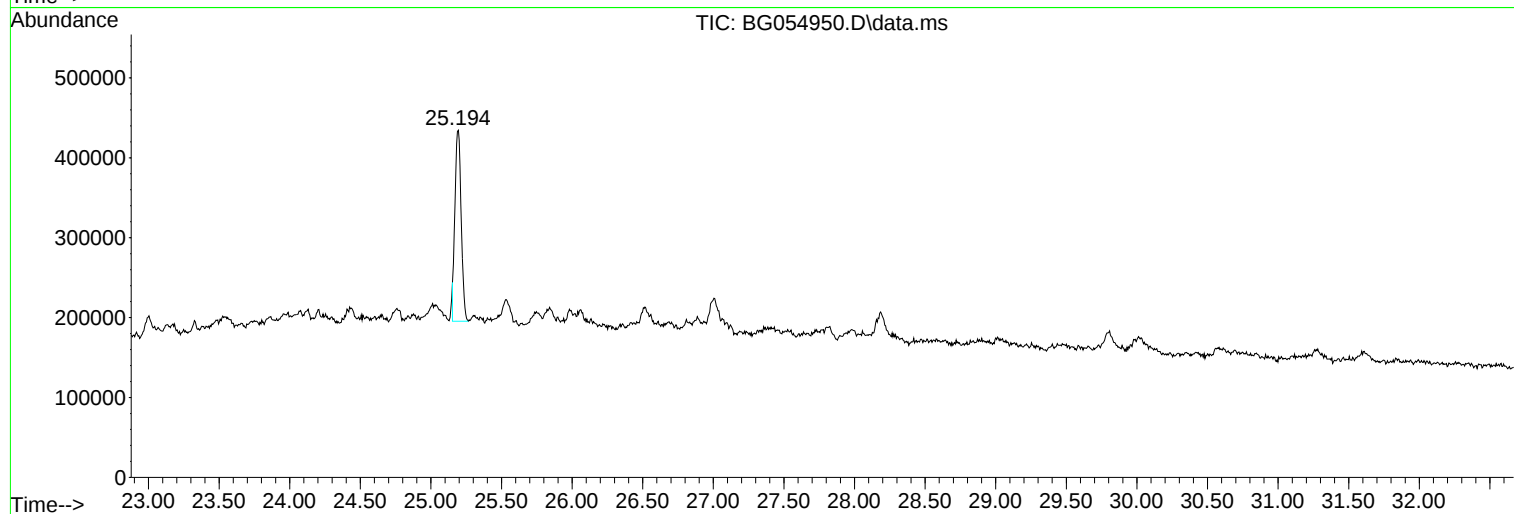
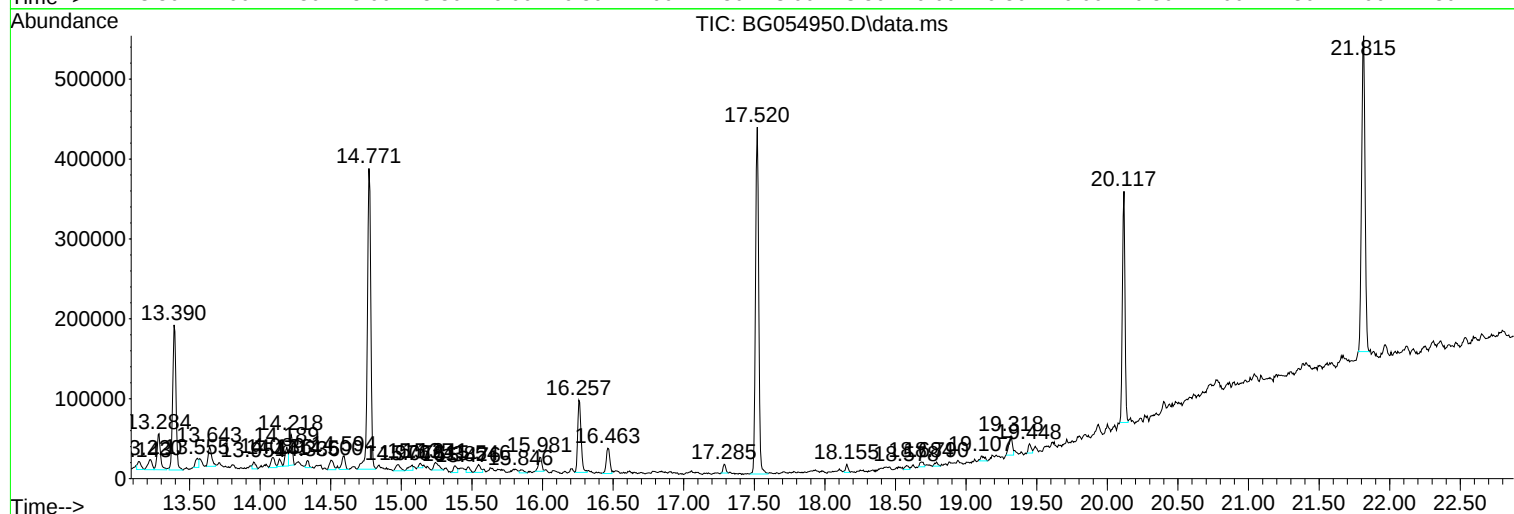
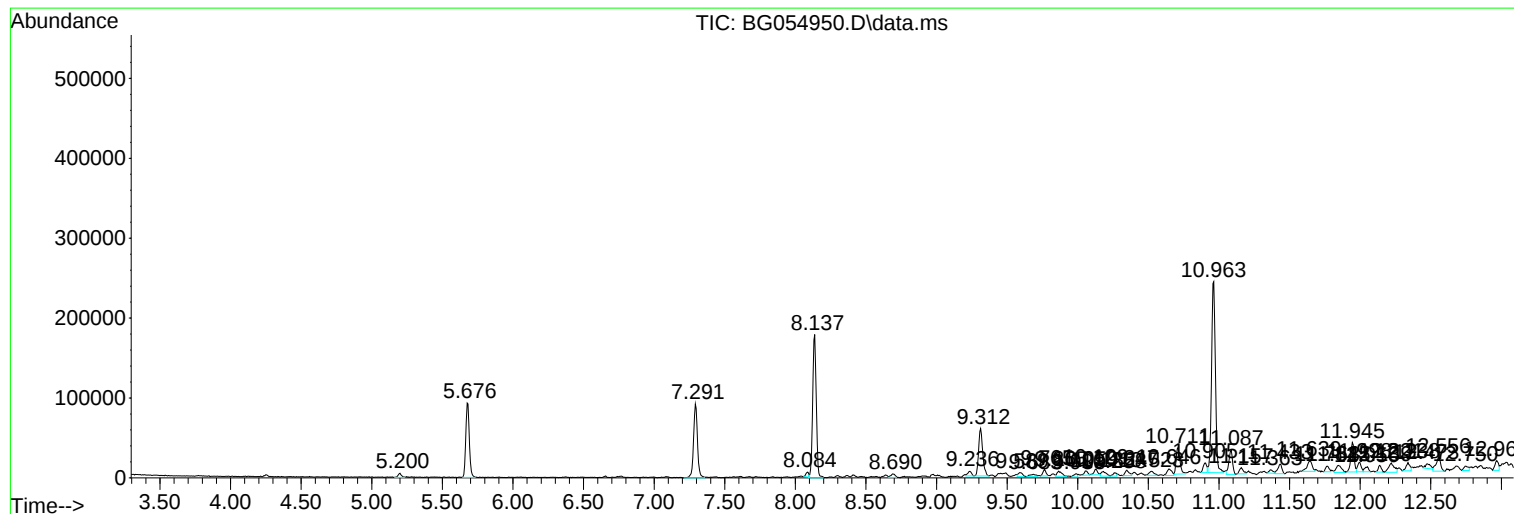
Sum of corrected areas: 6158639

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Instrument :
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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



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Data File : BG054950.D
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Operator : CG/JU
Sample : N4579-19 5X
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
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CHERRY-HILL-COMP-15

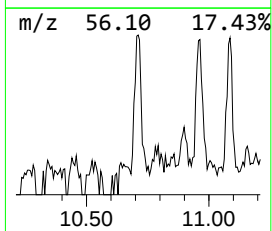
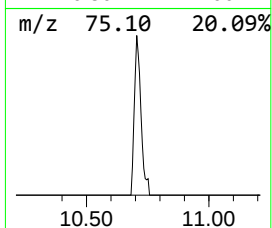
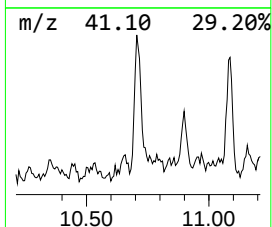
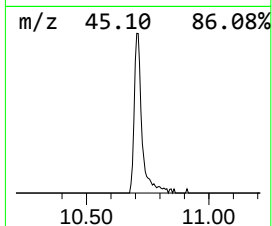
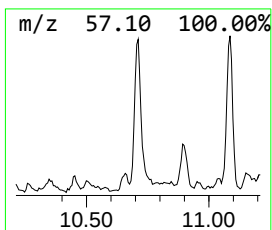
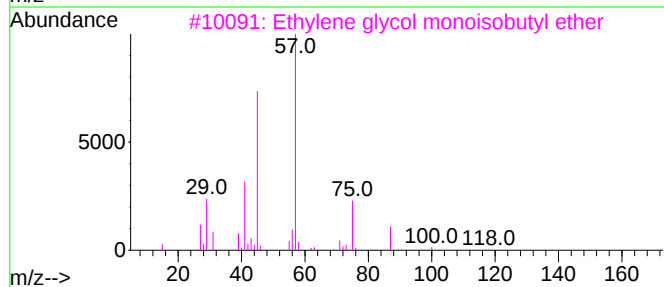
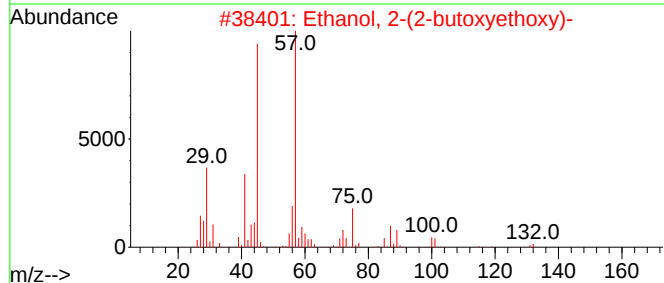
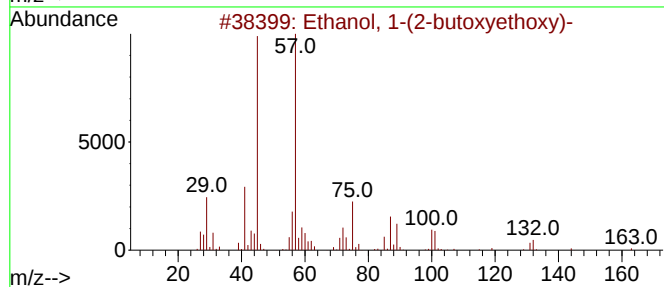
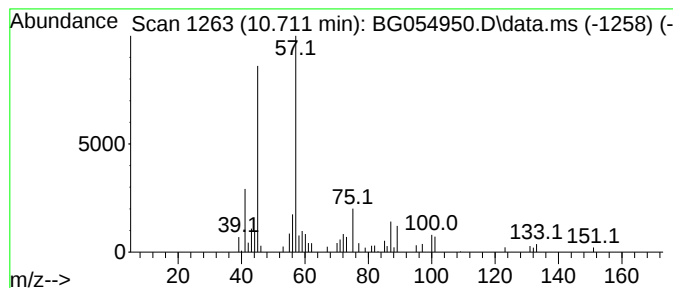
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG082522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Ethanol, 1-(2-butoxyethoxy)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.711	2.76 ng	63043	Naphthalene-d8	10.963

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	90
2			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
3			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	59
4			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	50
5			Butane, 1-(1-methylpropoxy)-	130	C8H18O	000999-65-5	47



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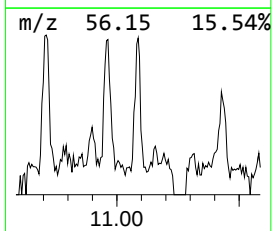
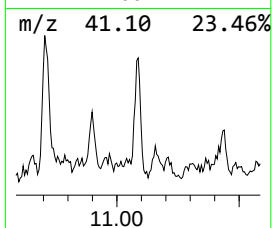
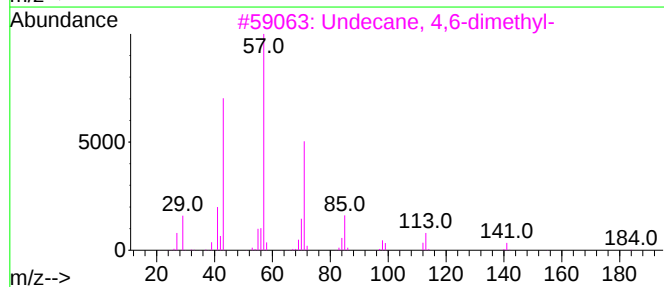
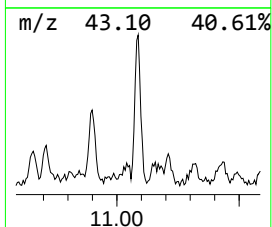
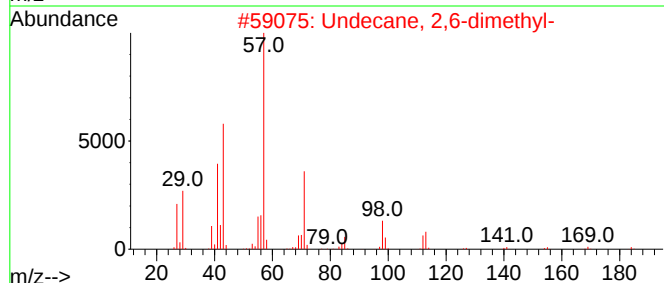
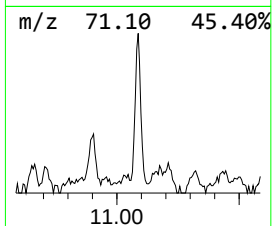
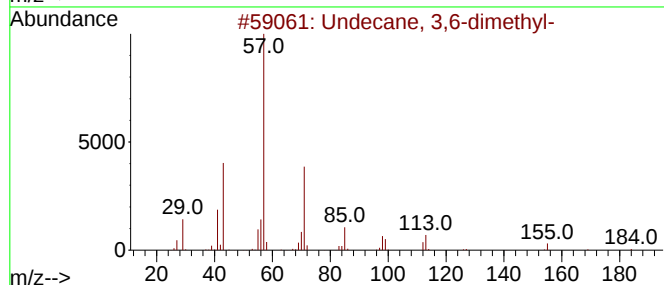
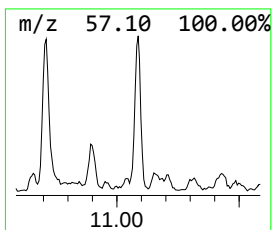
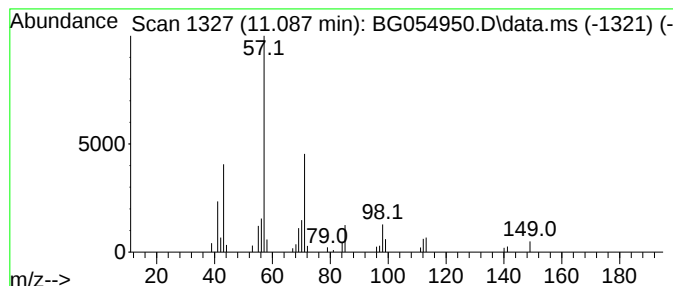
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG082522.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Undecane, 3,6-dimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.087	2.37 ng	54164	Naphthalene-d8	10.963

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Undecane, 3,6-dimethyl-	184	C13H28	017301-28-9	78
2			Undecane, 2,6-dimethyl-	184	C13H28	017301-23-4	78
3			Undecane, 4,6-dimethyl-	184	C13H28	017312-82-2	72
4			Dodecane, 2,7,10-trimethyl-	212	C15H32	074645-98-0	59
5			Dodecane, 6-methyl-	184	C13H28	006044-71-9	53



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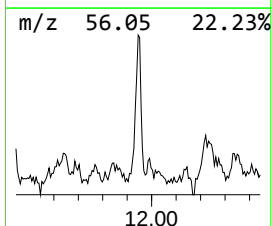
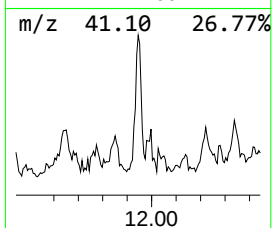
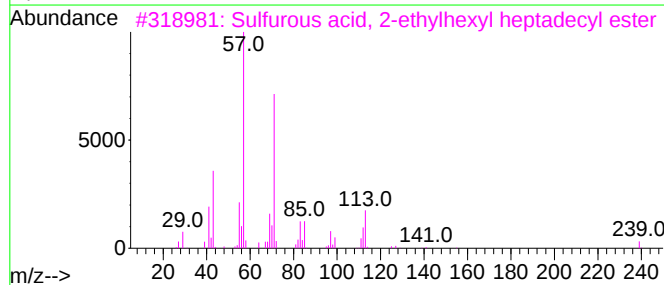
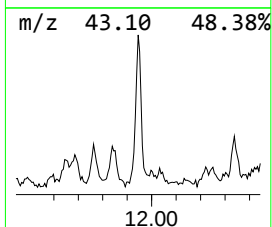
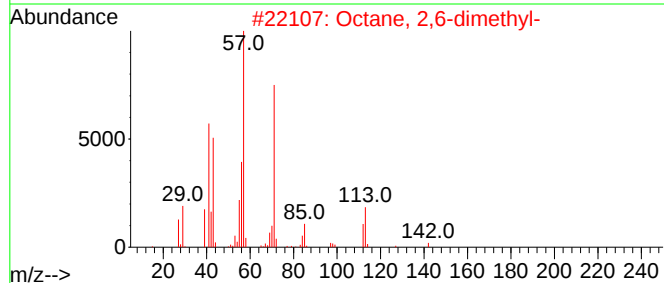
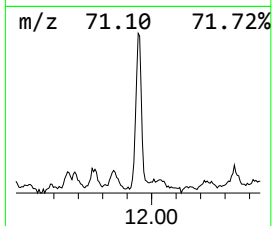
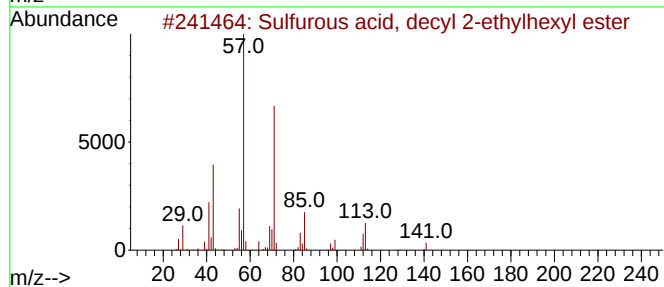
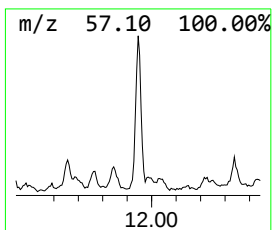
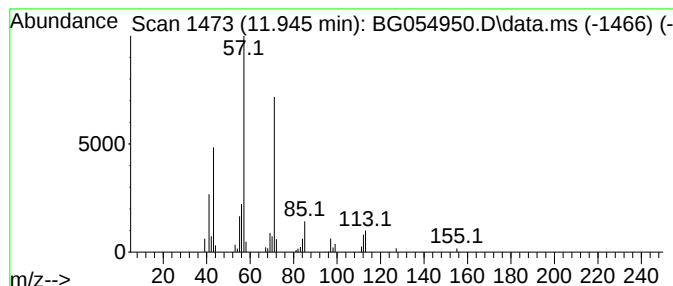
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Sulfurous acid, decyl 2-eth... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.945	2.71 ng	61907	Naphthalene-d8	10.963

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfurous acid, decyl 2-ethylhex...	334	C18H38O3S	1000309-19-3	72
2			Octane, 2,6-dimethyl-	142	C10H22	002051-30-1	64
3			Sulfurous acid, 2-ethylhexyl hep...	432	C25H52O3S	1000309-20-0	64
4			Octane, 3,6-dimethyl-	142	C10H22	015869-94-0	64
5			Undecane, 6,6-dimethyl-	184	C13H28	017312-76-4	59



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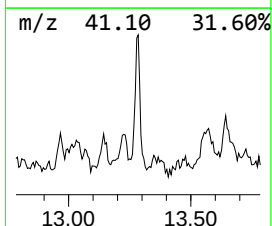
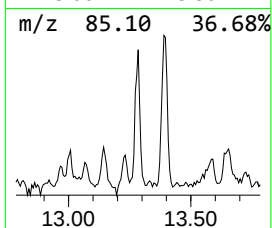
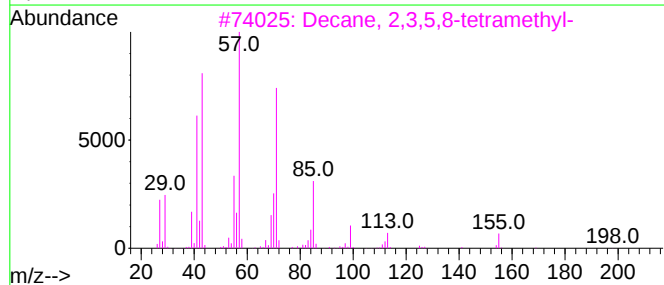
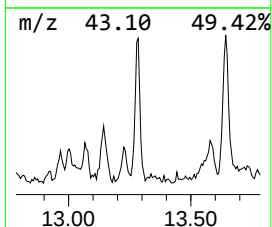
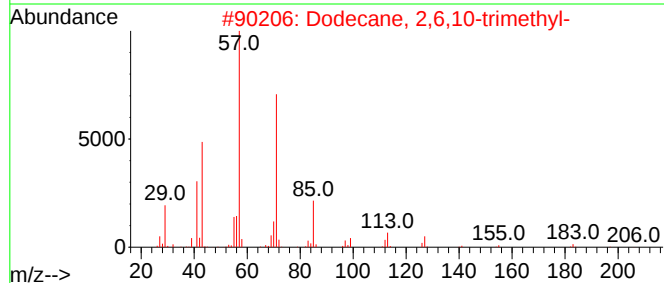
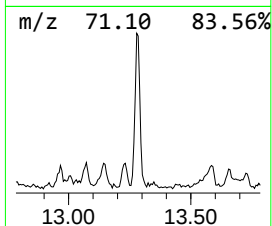
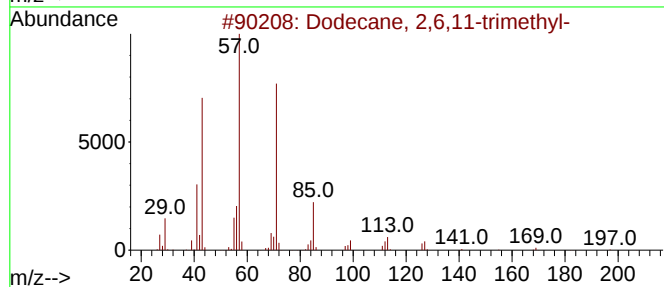
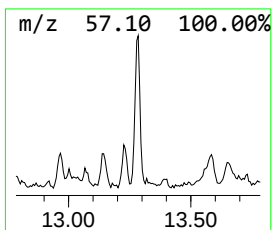
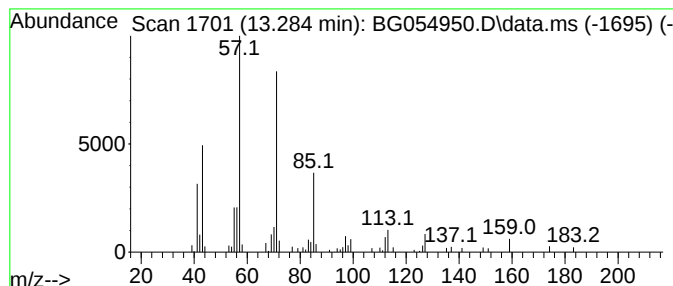
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG082522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Dodecane, 2,6,11-trimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.284	2.40 ng	75246	Acenaphthene-d10	14.771

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecane, 2,6,11-trimethyl-	212	C15H32	031295-56-4	90
2			Dodecane, 2,6,10-trimethyl-	212	C15H32	003891-98-3	83
3			Decane, 2,3,5,8-tetramethyl-	198	C14H30	192823-15-7	72
4			Nonane, 3-methyl-5-propyl-	184	C13H28	031081-18-2	72
5			Dodecane, 2,7,10-trimethyl-	212	C15H32	074645-98-0	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG091422\
Data File : BG054950.D
Acq On : 14 Sep 2022 19:27
Operator : CG/JU
Sample : N4579-19 5X
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
CHERRY-HILL-COMP-15

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
Ethanol, 1-(2-b...	10.711	2.8	ng	63043	2	10.963	457254	20.0
Undecane, 3,6-d...	11.087	2.4	ng	54164	2	10.963	457254	20.0
Sulfurous acid,...	11.945	2.7	ng	61907	2	10.963	457254	20.0
Dodecane, 2,6,1...	13.284	2.4	ng	75246	3	14.771	628010	20.0