

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082521\
 Data File : BF125219.D
 Acq On : 25 Aug 2021 20:22
 Operator : JU/CG
 Sample : M3467-01
 Misc :
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SAMPLE-11-(647.00)

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_F\METHODS\8270-BF081821.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF125219.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.204	15	20	28	rVB	893640	1134174	30.99%	3.197%
2	5.134	514	518	528	rVB	122097	147248	4.02%	0.415%
3	5.528	581	585	589	rBV	3704706	3659792	100.00%	10.318%
4	6.534	751	756	759	rBV	3761970	3365326	91.95%	9.488%
5	6.916	817	821	824	rBV	1408723	1225901	33.50%	3.456%
6	7.475	911	916	919	rBV	2559485	2205078	60.25%	6.217%
7	8.098	1019	1022	1035	rBV	122601	239980	6.56%	0.677%
8	8.198	1035	1039	1042	rBV	1674615	1440767	39.37%	4.062%
9	9.269	1217	1221	1224	rBV	4252933	3488135	95.31%	9.834%
10	9.810	1309	1313	1316	rBV	57977	52419	1.43%	0.148%
11	9.951	1333	1337	1340	rBV	1642698	1380263	37.71%	3.891%
12	10.733	1467	1470	1474	rBV	2104881	1912798	52.27%	5.393%
13	10.986	1509	1513	1518	rBV6	38726	52500	1.43%	0.148%
14	11.439	1586	1590	1592	rBV	1419525	1309560	35.78%	3.692%
15	11.457	1592	1593	1597	rVV	169738	124925	3.41%	0.352%
16	11.510	1600	1602	1604	rBV	66581	50906	1.39%	0.144%
17	11.951	1674	1677	1682	rBV2	299483	308418	8.43%	0.869%
18	12.051	1691	1694	1696	rBV	53380	50229	1.37%	0.142%
19	12.257	1727	1729	1733	rVB	62451	52884	1.45%	0.149%
20	12.486	1766	1768	1772	rBV3	37470	40782	1.11%	0.115%
21	12.568	1780	1782	1785	rBV	48635	44156	1.21%	0.124%
22	12.651	1793	1796	1800	rBV	1110476	931503	25.45%	2.626%
23	12.739	1808	1811	1815	rBV2	190888	176779	4.83%	0.498%
24	12.880	1829	1835	1839	rBV	1019872	998898	27.29%	2.816%
25	13.021	1855	1859	1862	rBV	3977127	3349096	91.51%	9.442%
26	13.204	1888	1890	1893	rVB	97272	87039	2.38%	0.245%
27	13.404	1922	1924	1926	rVB2	76603	51323	1.40%	0.145%
28	13.710	1974	1976	1979	rBV	168528	159266	4.35%	0.449%
29	13.857	1999	2001	2002	rBV	91859	71981	1.97%	0.203%
30	14.080	2034	2039	2041	rBV2	1631260	1972178	53.89%	5.560%
31	14.104	2041	2043	2049	rVB	797946	654814	17.89%	1.846%
32	15.133	2214	2218	2222	rBV	820134	1305769	35.68%	3.681%
33	15.209	2228	2231	2234	rVB2	209188	248596	6.79%	0.701%
34	15.445	2268	2271	2278	rVB	454283	589855	16.12%	1.663%
35	15.509	2279	2282	2289	rVB	471901	610768	16.69%	1.722%
36	15.580	2289	2294	2297	rBV	1044109	1403722	38.36%	3.957%

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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_F\METHODS\8270-BF081821.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	15.809	2331	2333	2338	rVB3	200841	223032	6.09%	0.629%
38	17.545	2624	2628	2635	rVB	187835	350161	9.57%	0.987%

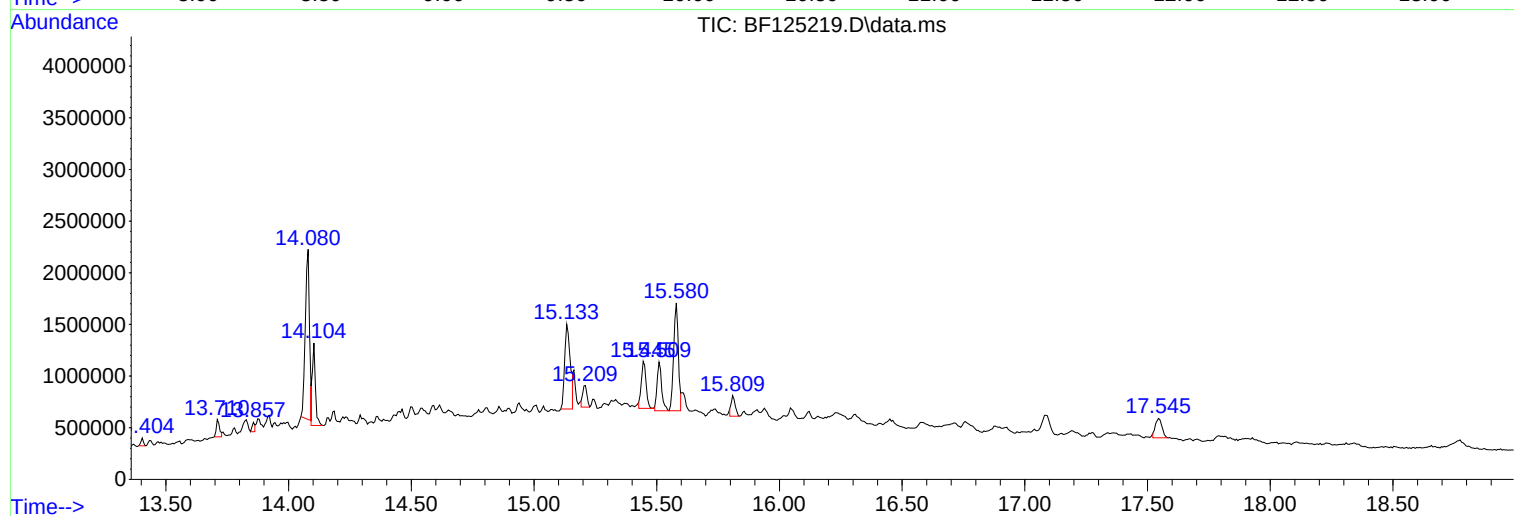
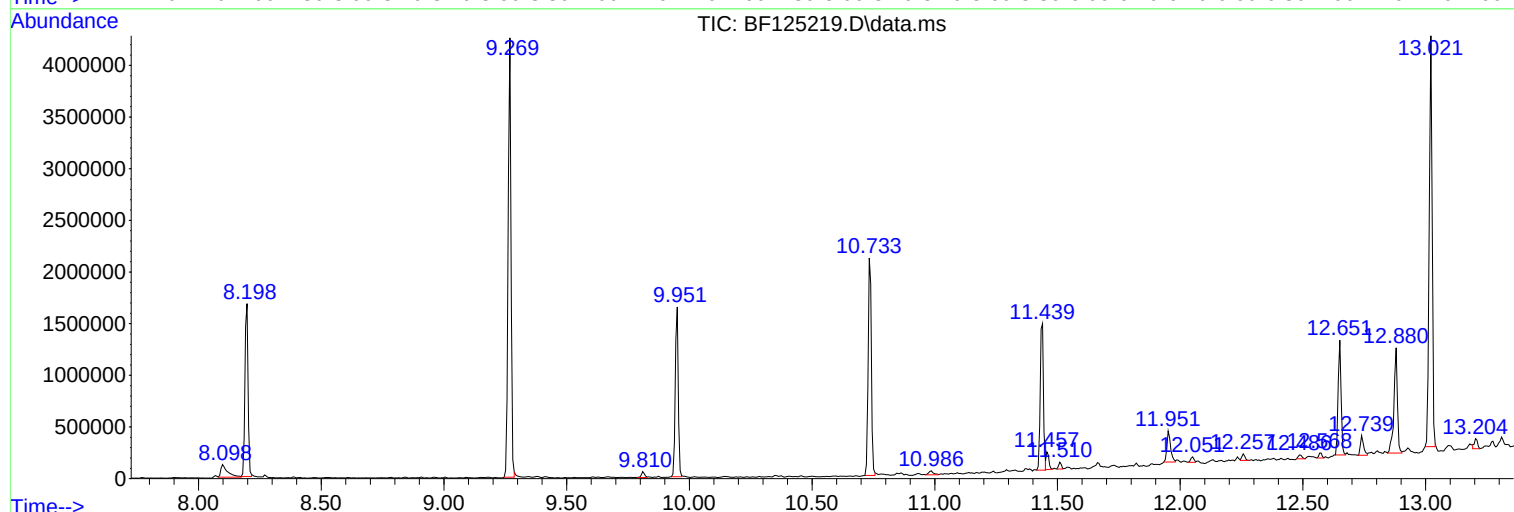
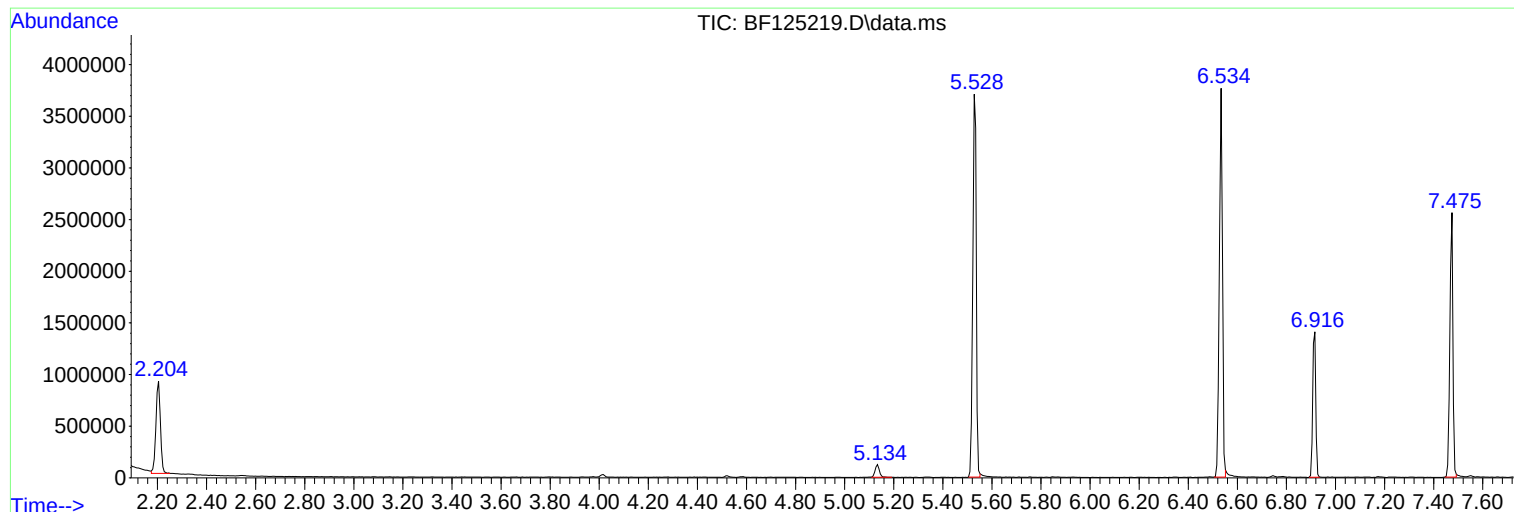
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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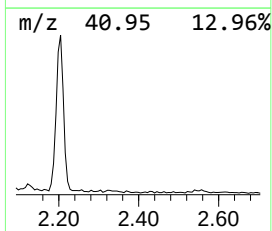
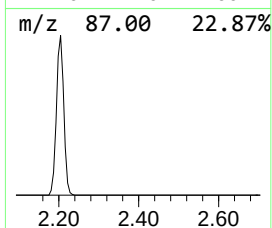
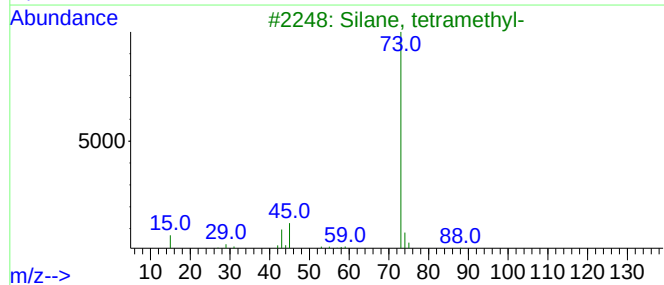
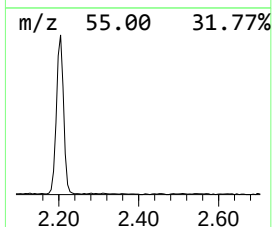
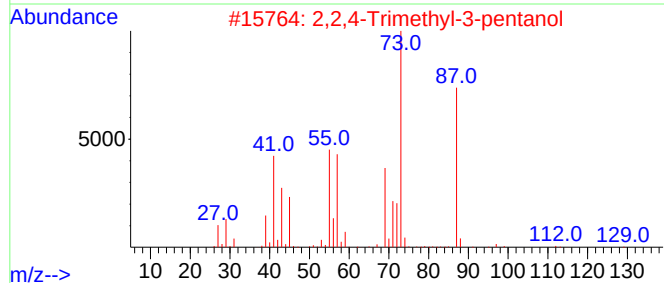
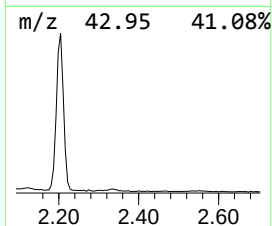
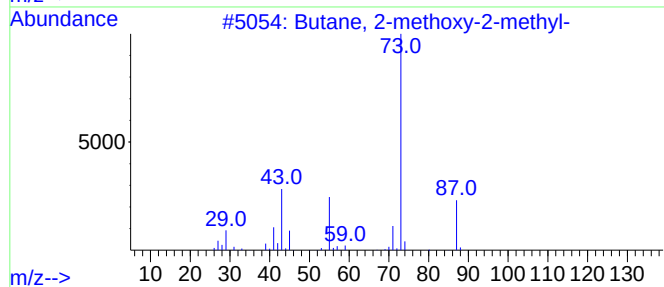
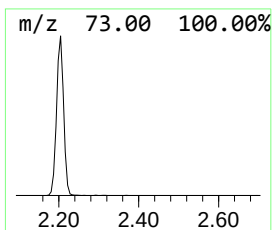
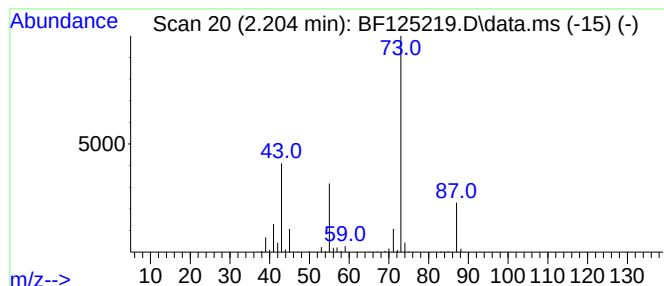
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.204	18.50 ng	1134170	1,4-Dichlorobenzene-d4	6.916

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	39
3			Silane, tetramethyl-	88	C4H12Si	000075-76-3	17
4			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
5			N-Ethylformamide	73	C3H7NO	000627-45-2	9



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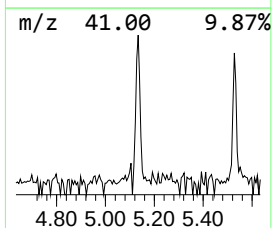
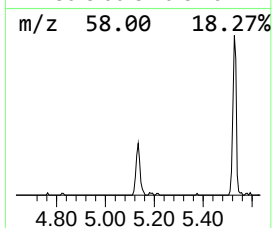
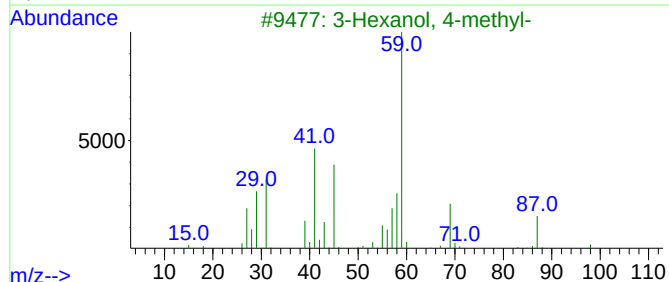
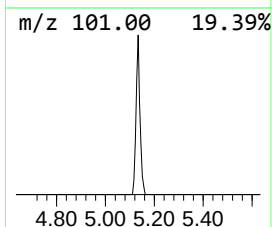
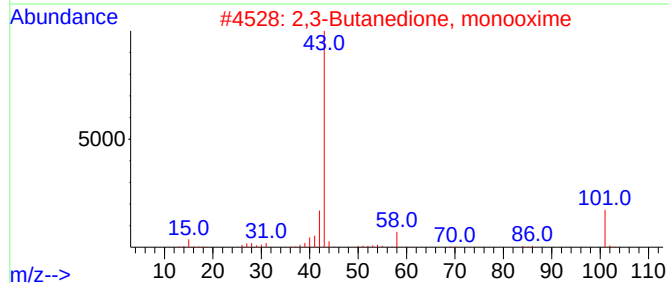
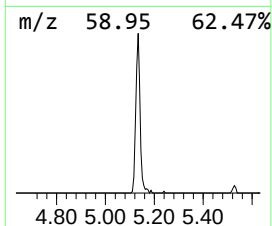
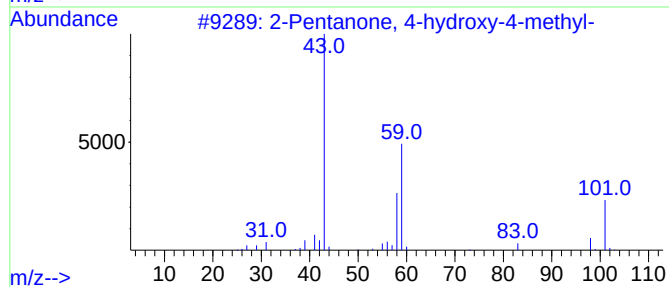
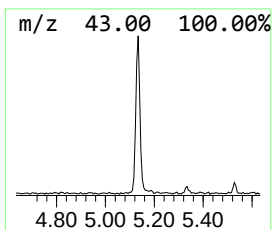
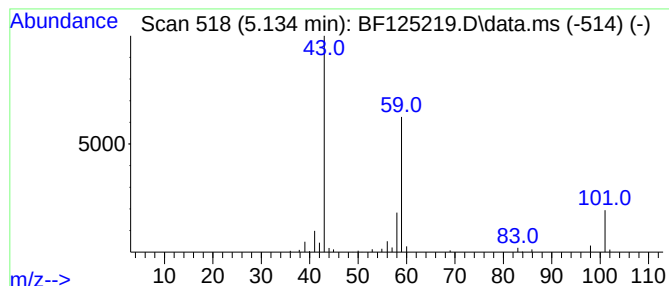
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TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.134	2.40 ng	147248	1,4-Dichlorobenzene-d4	6.916

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	32
3			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
4			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5			Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9



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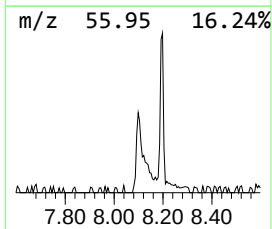
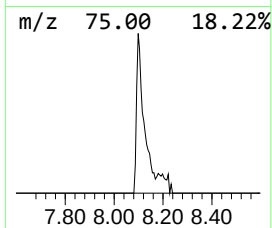
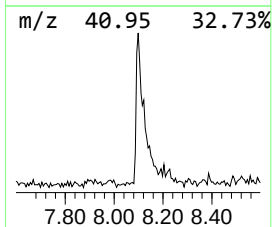
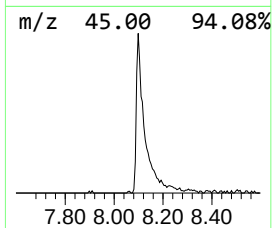
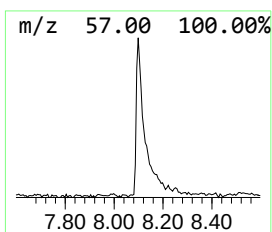
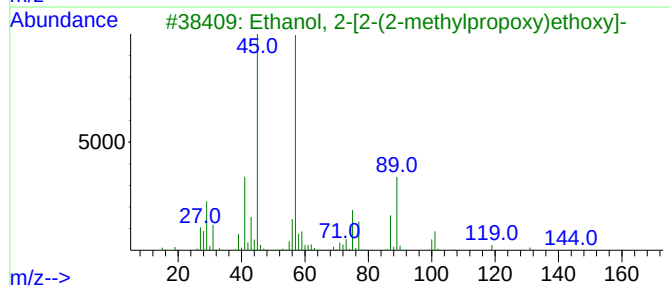
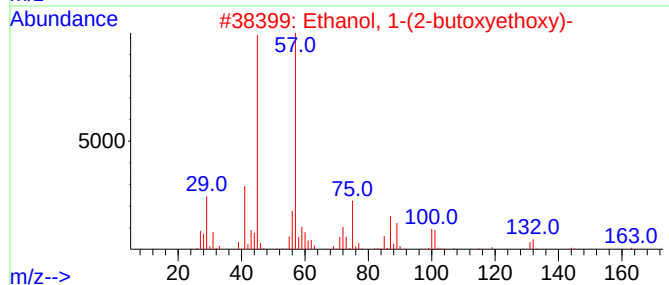
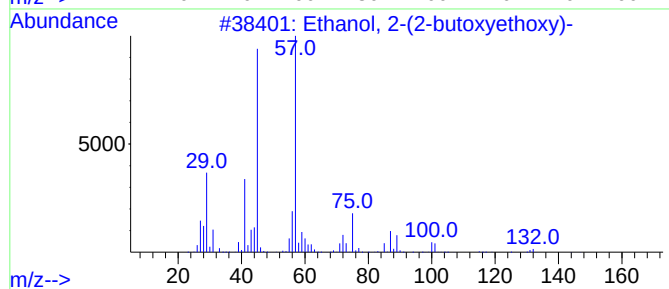
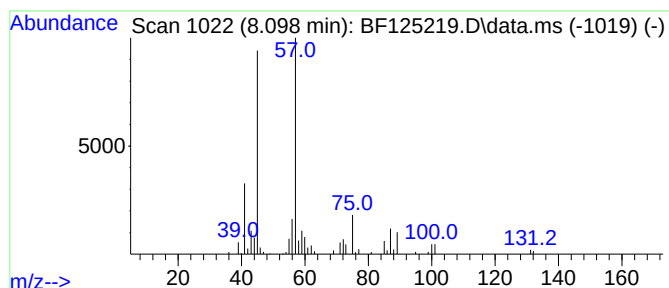
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.098	3.33 ng	239980	Naphthalene-d8	8.198

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2			Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	83
3			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	78
4			2-Propanol, 1-butoxy-	132	C7H16O2	005131-66-8	53
5			Propanoic acid, 2-(methoxymethoxy)-	134	C5H10O4	081327-29-9	50



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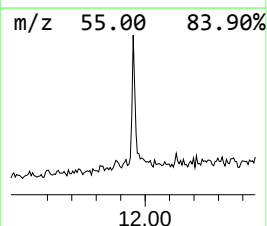
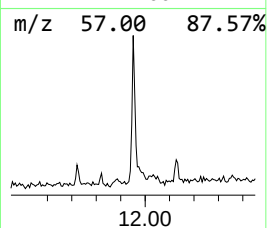
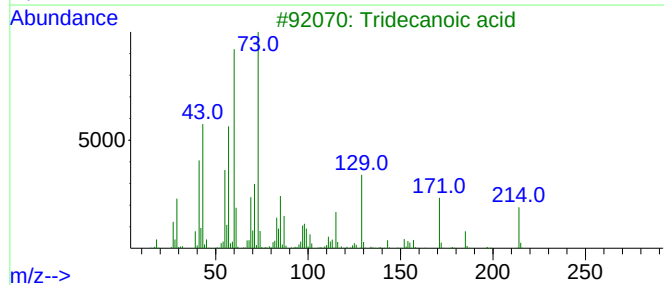
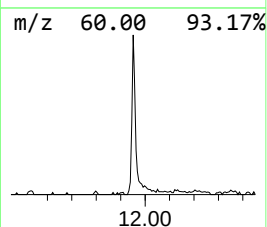
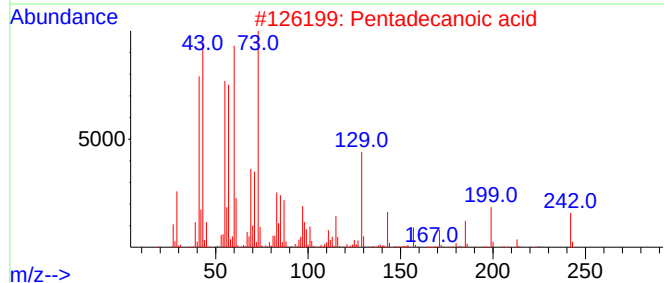
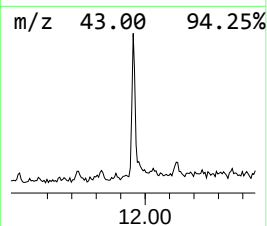
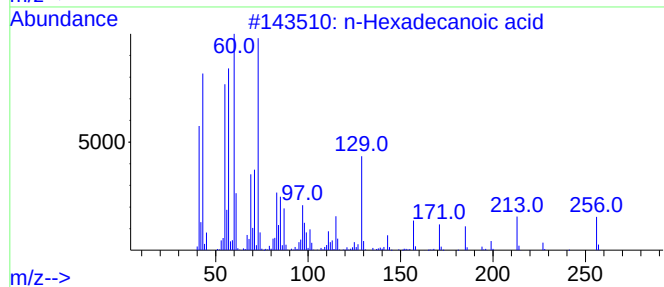
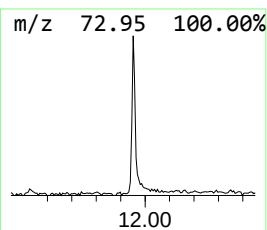
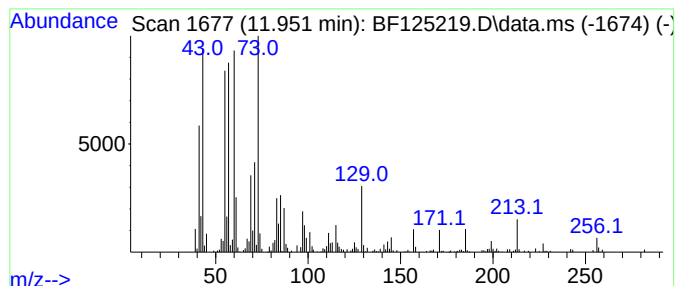
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.951	4.71 ng	308418	Phenanthrene-d10	11.439

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	95
3			Tridecanoic acid	214	C13H26O2	000638-53-9	87
4			Dodecanoic acid	200	C12H24O2	000143-07-7	83
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	74



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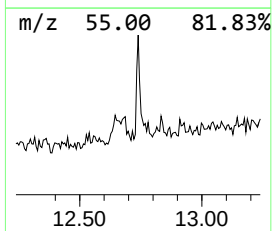
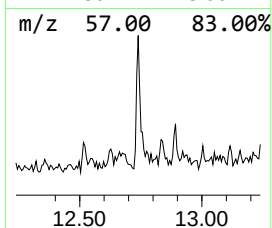
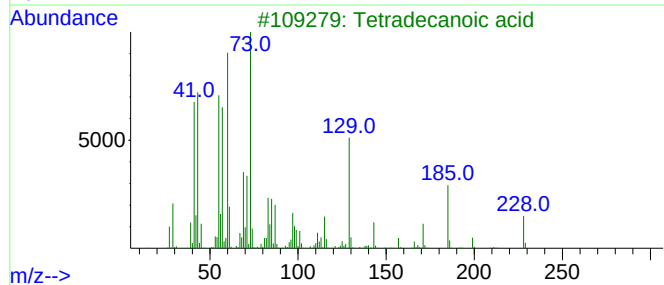
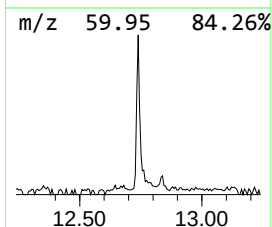
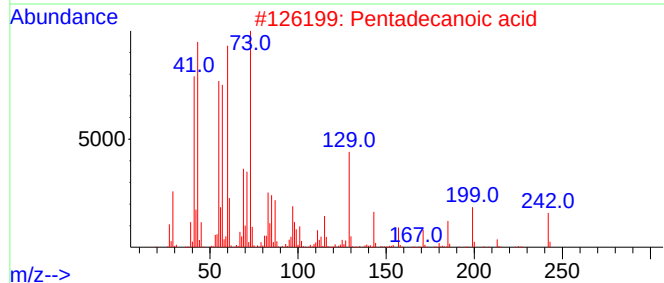
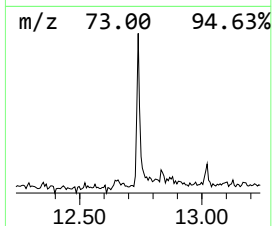
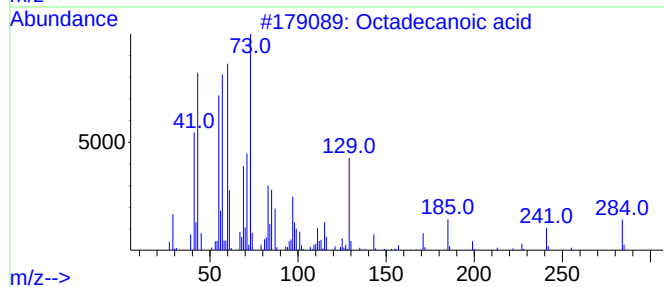
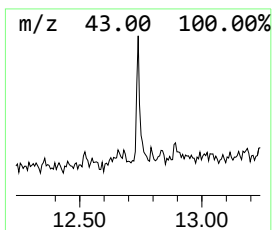
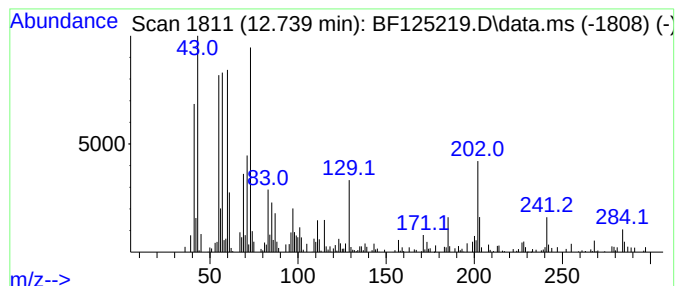
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TIC Integration Parameters: LSCINT.P

Peak Number 5 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.739	2.70 ng	176779	Phenanthrene-d10	11.439

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	94
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	83
4			Dodecanoic acid	200	C12H24O2	000143-07-7	78
5			8-Methylnonanoic acid	172	C10H20O2	005963-14-4	70



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082521\
Data File : BF125219.D
Acq On : 25 Aug 2021 20:22
Operator : JU/CG
Sample : M3467-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SAMPLE-11-(647.00)

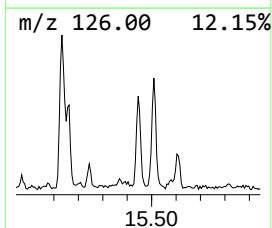
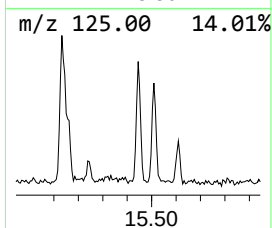
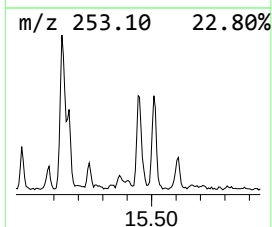
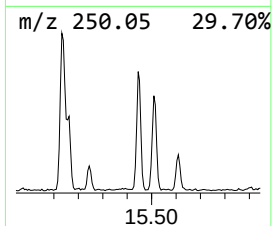
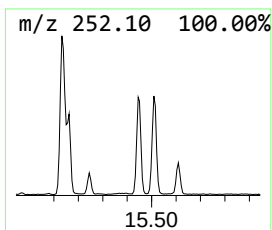
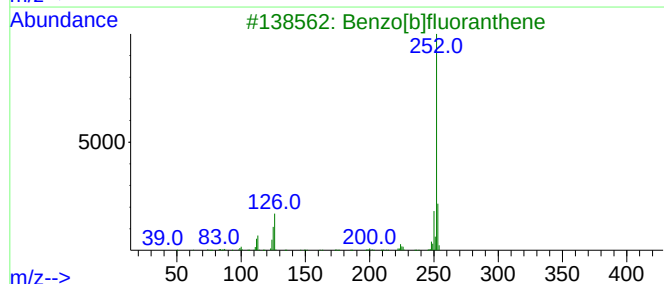
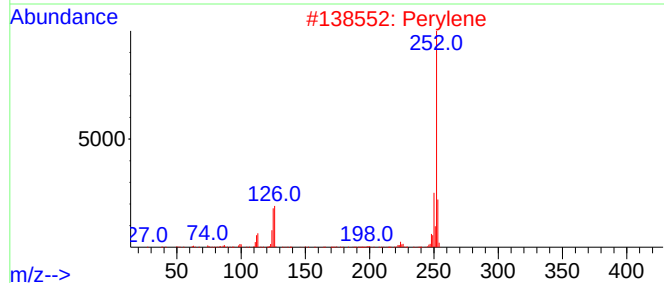
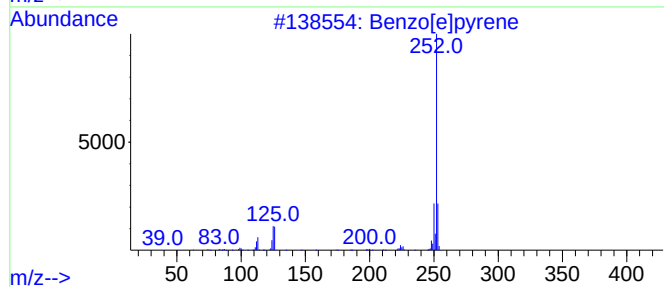
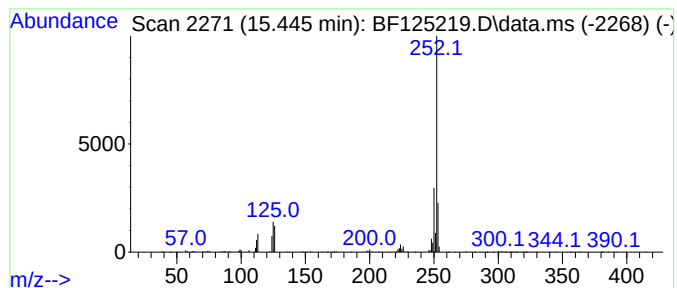
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Benzo[e]pyrene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.445	8.40 ng	589855	Perylene-d12	15.580

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[e]pyrene	252	C20H12	000192-97-2	98
2			Perylene	252	C20H12	000198-55-0	93
3			Benzo[b]fluoranthene	252	C20H12	000205-99-2	93
4			Benzo[a]pyrene	252	C20H12	000050-32-8	93
5			Benzo[k]fluoranthene	252	C20H12	000207-08-9	93



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082521\
Data File : BF125219.D
Acq On : 25 Aug 2021 20:22
Operator : JU/CG
Sample : M3467-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SAMPLE-11-(647.00)

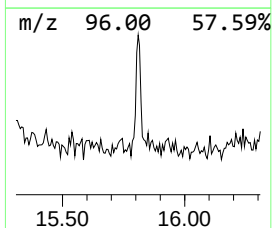
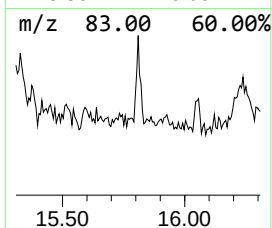
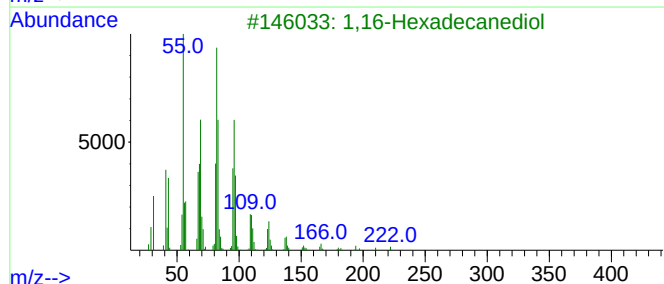
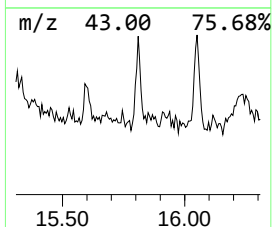
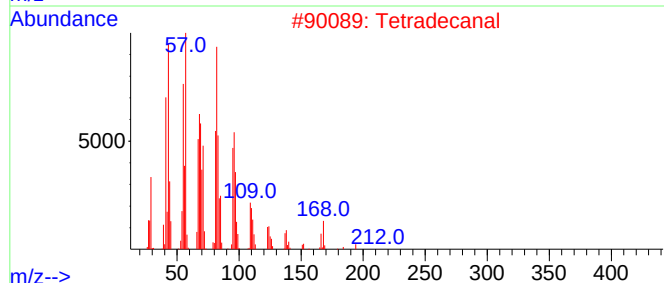
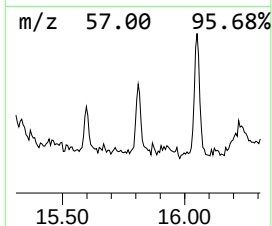
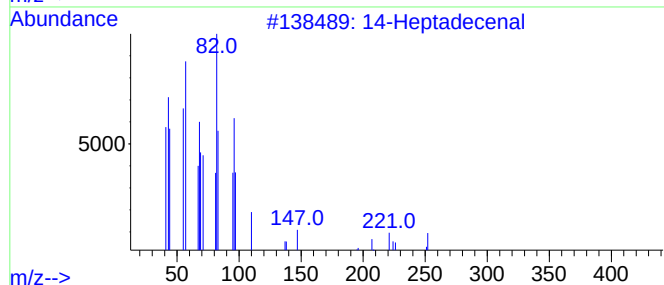
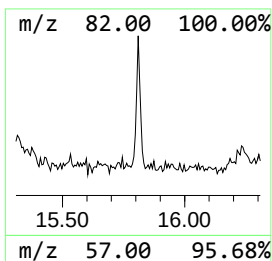
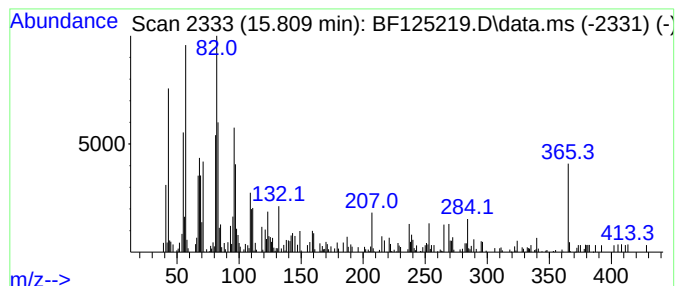
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 14-Heptadecenal Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.809	3.18 ng	223032	Perylene-d12	15.580

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			14-Heptadecenal	252	C17H32O	1010144-58-0	83
2			Tetradecanal	212	C14H28O	000124-25-4	52
3			1,16-Hexadecanediol	258	C16H34O2	007735-42-4	52
4			11-Tetradecyn-1-ol acetate	252	C16H28O2	033925-72-3	52
5			Hexacosanal	380	C26H52O	026627-85-0	50



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Operator : JU/CG
Sample : M3467-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SAMPLE-11-(647.00)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.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
Butane, 2-metho...	2.204	18.5	ng	1134170	1	6.916	1225900	20.0
2-Pentanone, 4-...	5.134	2.4	ng	147248	1	6.916	1225900	20.0
Ethanol, 2-(2-b...	8.098	3.3	ng	239980	2	8.198	1440770	20.0
n-Hexadecanoic ...	11.951	4.7	ng	308418	4	11.439	1309560	20.0
Octadecanoic acid	12.739	2.7	ng	176779	4	11.439	1309560	20.0
Benzo[e]pyrene	15.445	8.4	ng	589855	6	15.580	1403720	20.0
14-Heptadecenal	15.809	3.2	ng	223032	6	15.580	1403720	20.0