

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082721\
 Data File : BF125256.D
 Acq On : 27 Aug 2021 16:25
 Operator : JU/CG
 Sample : M3548-01
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 VNJ-235

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: BF125256.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.199	13	19	26	rVB	1175884	1498377	35.41%	4.394%
2	5.528	581	585	588	rBV	3901225	3667665	86.67%	10.755%
3	6.534	751	756	759	rBV	3664091	3714768	87.78%	10.893%
4	6.910	817	820	824	rBV	1375369	1131463	26.74%	3.318%
5	7.475	911	916	919	rBV	2736825	2406916	56.87%	7.058%
6	8.104	1019	1023	1032	rBV2	57988	162362	3.84%	0.476%
7	8.192	1035	1038	1042	rBV	1600782	1450112	34.27%	4.252%
8	9.269	1217	1221	1224	rBV	5260507	4232002	100.00%	12.409%
9	9.951	1333	1337	1340	rBV	1834324	1670449	39.47%	4.898%
10	10.251	1382	1388	1394	rBV	71503	158654	3.75%	0.465%
11	10.739	1466	1471	1474	rBV	2944305	2855631	67.48%	8.373%
12	10.857	1487	1491	1494	rVB2	60356	75248	1.78%	0.221%
13	11.327	1567	1571	1576	rVB3	36878	55365	1.31%	0.162%
14	11.433	1586	1589	1592	rBV	1825361	1710147	40.41%	5.015%
15	11.457	1592	1593	1596	rVB	188108	122947	2.91%	0.361%
16	11.951	1672	1677	1683	rBV2	451695	552366	13.05%	1.620%
17	12.045	1691	1693	1696	rBV2	48032	50792	1.20%	0.149%
18	12.157	1709	1712	1714	rBV	63438	50583	1.20%	0.148%
19	12.263	1727	1730	1733	rVB2	65631	59447	1.40%	0.174%
20	12.651	1793	1796	1800	rBV	300476	260974	6.17%	0.765%
21	12.686	1800	1802	1805	rBV2	70000	68300	1.61%	0.200%
22	12.739	1808	1811	1817	rBV2	213536	231820	5.48%	0.680%
23	12.880	1829	1835	1840	rBV	254357	309808	7.32%	0.908%
24	13.021	1855	1859	1862	rBV	4221447	3752902	88.68%	11.004%
25	13.980	2017	2022	2023	rBV5	69107	115698	2.73%	0.339%
26	14.074	2034	2038	2041	rBV	1287755	1257171	29.71%	3.686%
27	14.098	2041	2042	2045	rVB	115588	86786	2.05%	0.254%
28	14.463	2101	2104	2108	rVB3	54077	66861	1.58%	0.196%
29	14.533	2114	2116	2118	rBV	56797	50469	1.19%	0.148%
30	15.004	2193	2196	2199	rVB	82919	77851	1.84%	0.228%
31	15.127	2214	2217	2221	rBV	125156	202979	4.80%	0.595%
32	15.204	2226	2230	2233	rVB	143773	169200	4.00%	0.496%
33	15.439	2268	2270	2277	rVB	84817	113134	2.67%	0.332%
34	15.504	2279	2281	2288	rVB	98168	123269	2.91%	0.361%
35	15.574	2288	2293	2302	rBV	929049	1284635	30.36%	3.767%
36	15.804	2329	2332	2337	rVB3	71398	95446	2.26%	0.280%

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082721\
Data File : BF125256.D
Acq On : 27 Aug 2021 16:25
Operator : JU/CG
Sample : M3548-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VNJ-235

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	16.045	2368	2373	2377	rVB	141700	210818	4.98%	0.618%
----	--------	------	------	------	-----	--------	--------	-------	--------

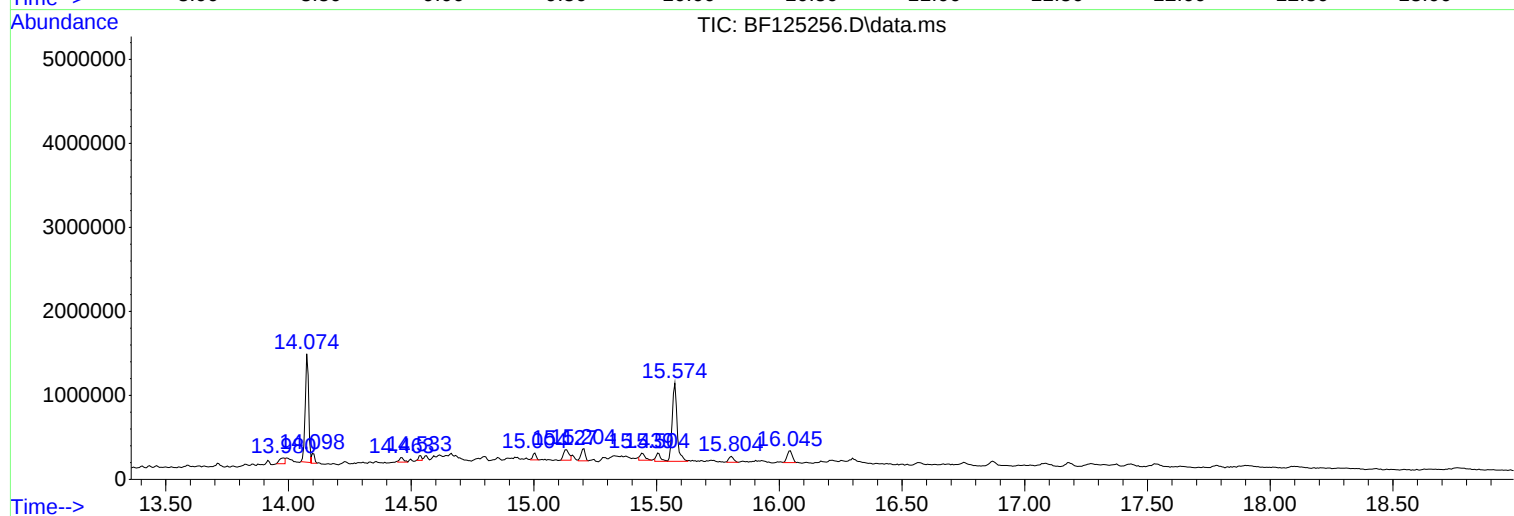
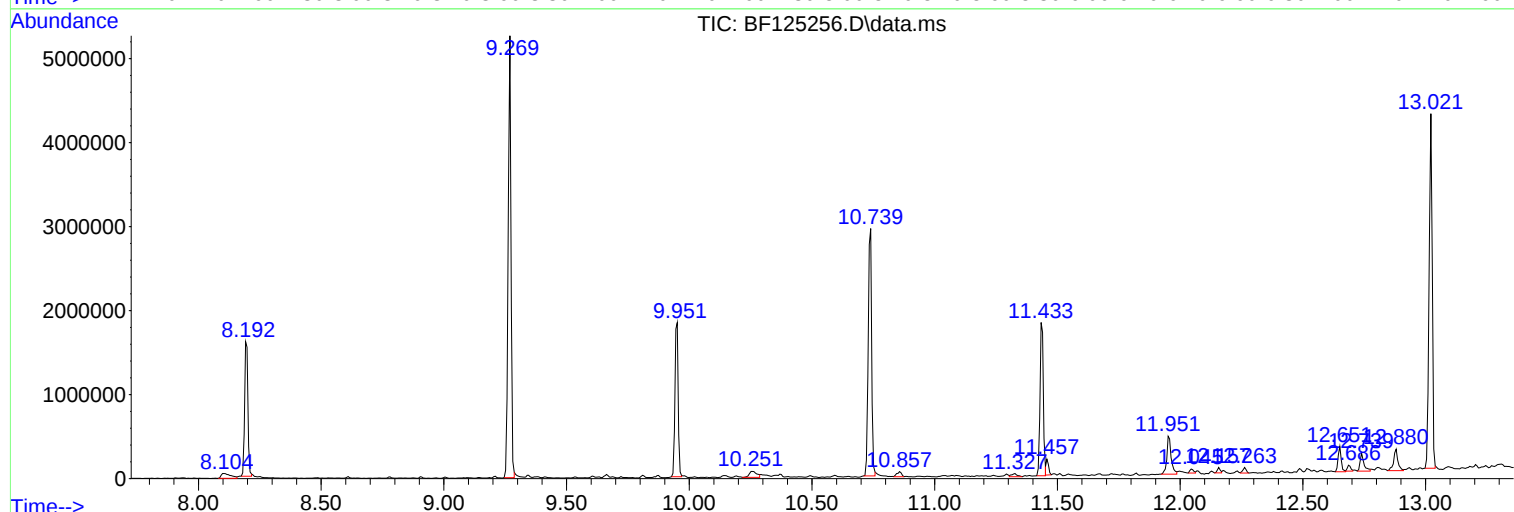
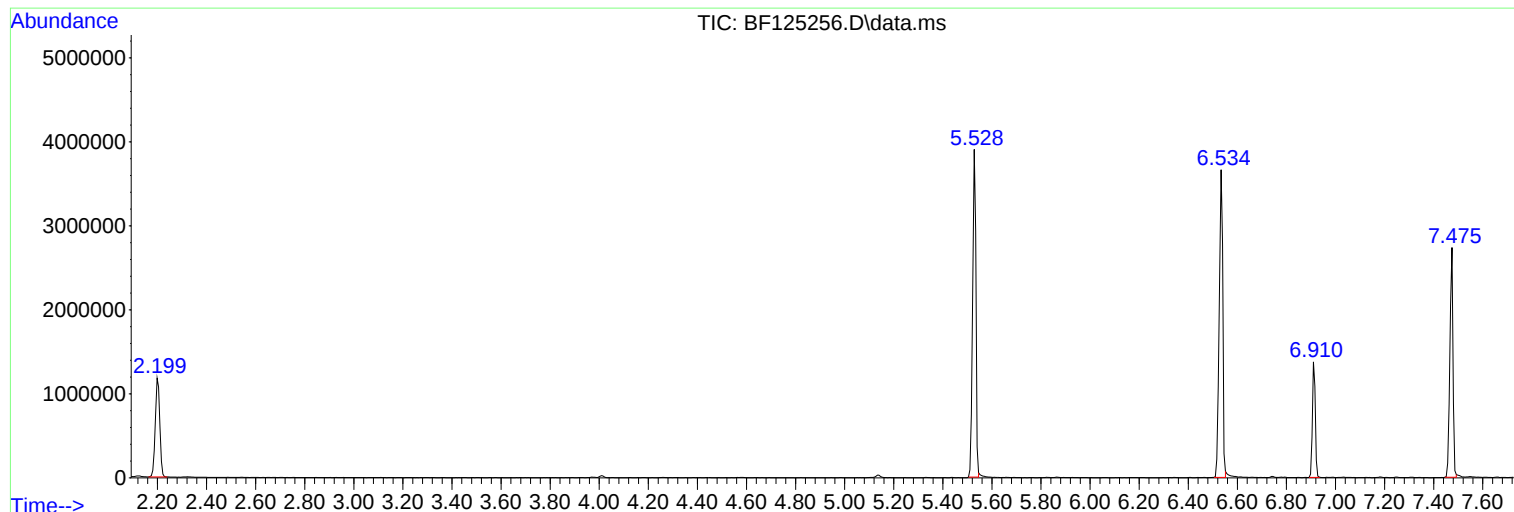
Sum of corrected areas: 34103415

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082721\
Data File : BF125256.D
Acq On : 27 Aug 2021 16:25
Operator : JU/CG
Sample : M3548-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VNJ-235

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082721\
Data File : BF125256.D
Acq On : 27 Aug 2021 16:25
Operator : JU/CG
Sample : M3548-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VNJ-235

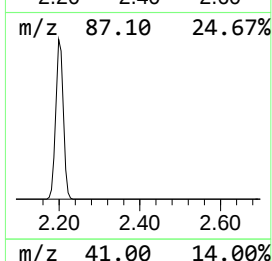
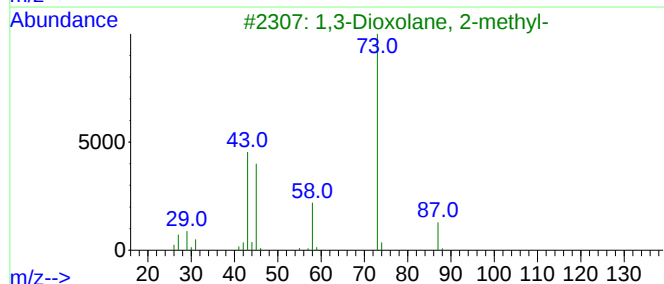
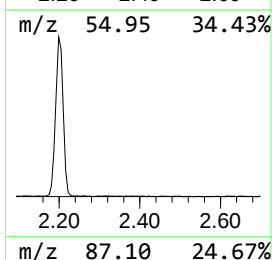
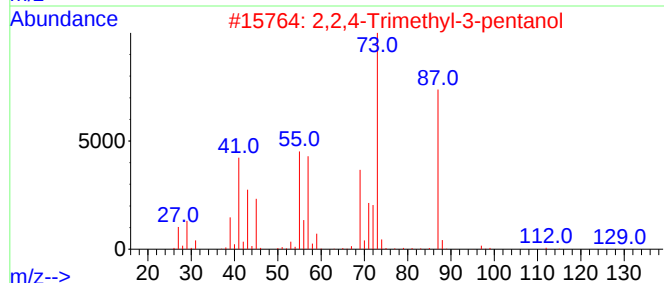
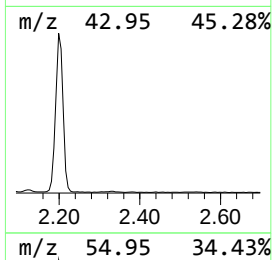
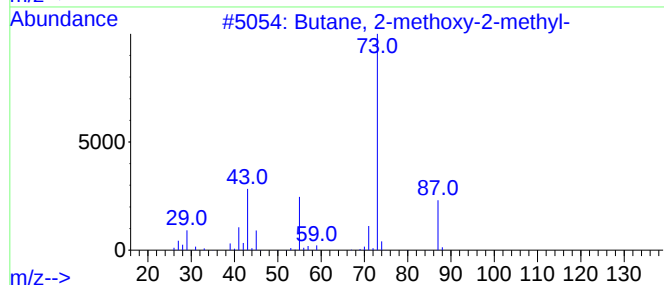
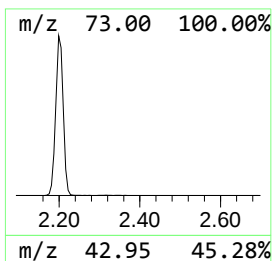
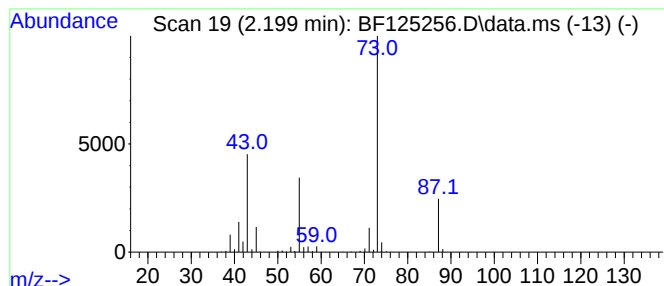
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.199	26.49 ng	1498380	1,4-Dichlorobenzene-d4	6.910

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			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	37
4			Silane, tetramethyl-	88	C4H12Si	000075-76-3	35
5			3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082721\
Data File : BF125256.D
Acq On : 27 Aug 2021 16:25
Operator : JU/CG
Sample : M3548-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VNJ-235

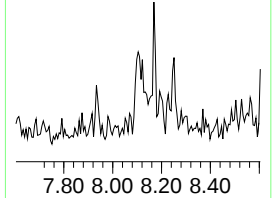
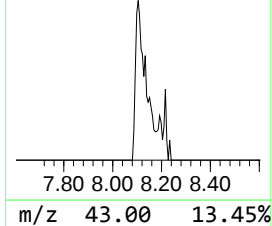
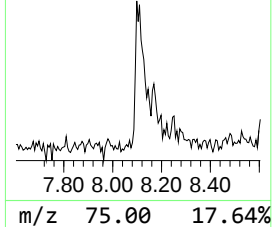
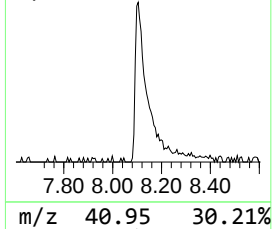
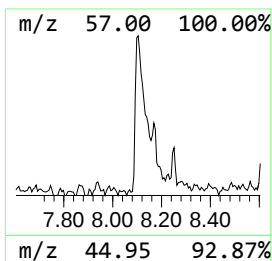
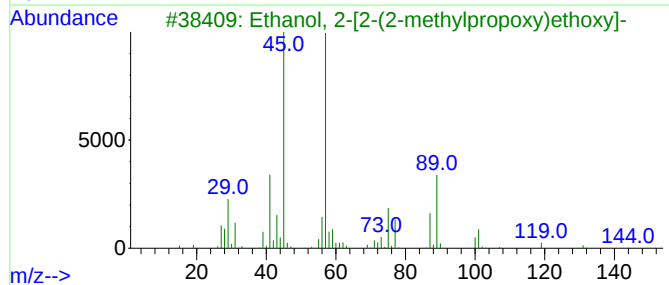
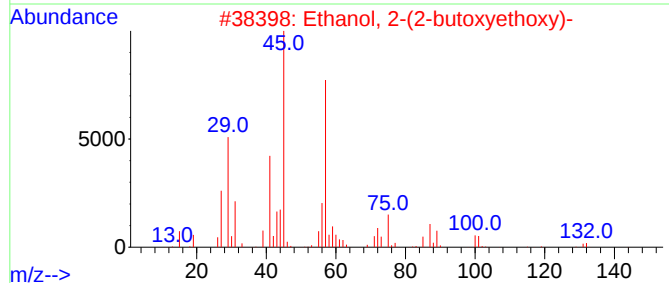
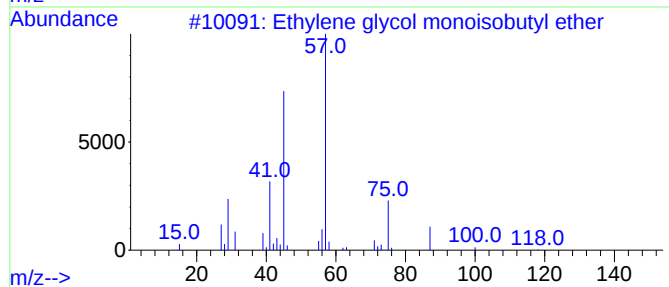
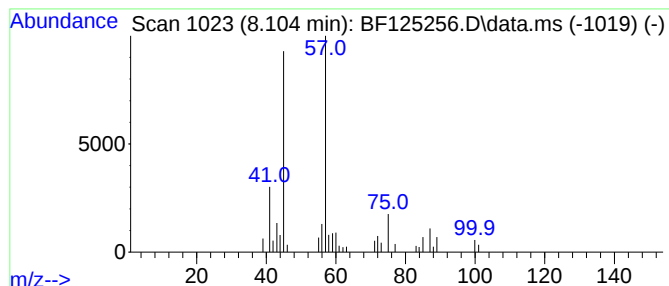
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Ethylene glycol monoisobuty... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.104	2.24 ng	162362	Naphthalene-d8	8.192

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	64
2			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	64
3			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	64
4			Ethylene glycol diglycidyl ether	174	C8H14O4	002224-15-9	45
5			Butane, 1-(1-methylpropoxy)-	130	C8H18O	000999-65-5	42



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082721\
Data File : BF125256.D
Acq On : 27 Aug 2021 16:25
Operator : JU/CG
Sample : M3548-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VNJ-235

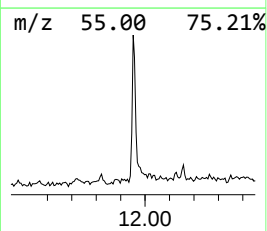
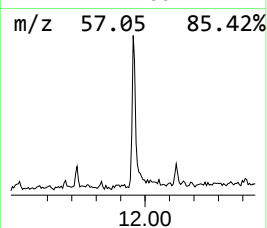
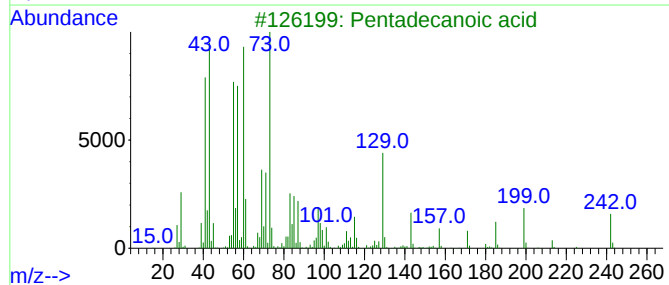
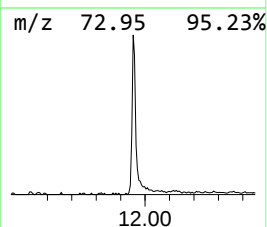
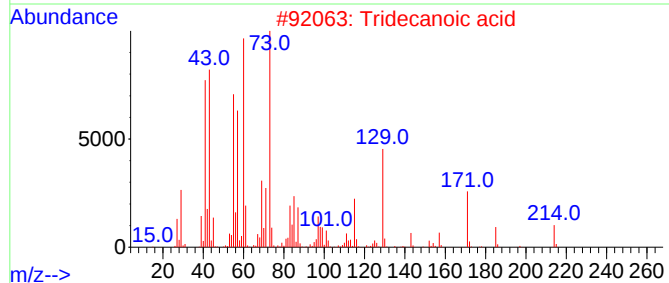
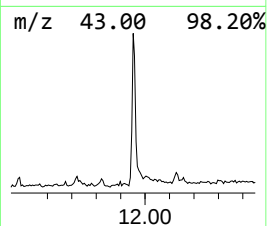
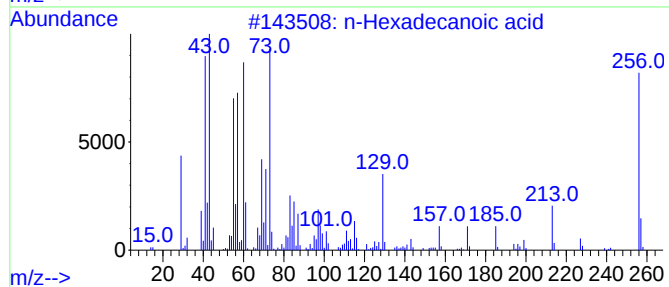
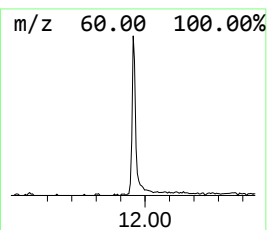
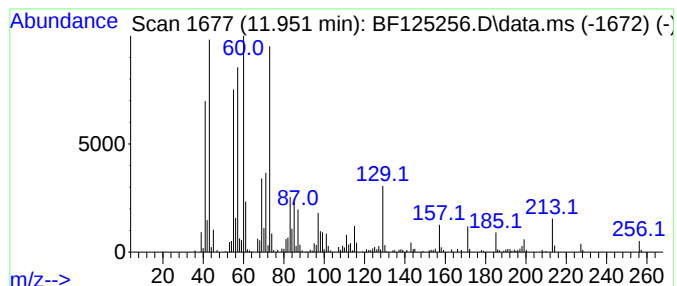
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.951	6.46 ng	552366	Phenanthrene-d10	11.433

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2			Tridecanoic acid	214	C13H26O2	000638-53-9	91
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5			n-Decanoic acid	172	C10H20O2	000334-48-5	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082721\
Data File : BF125256.D
Acq On : 27 Aug 2021 16:25
Operator : JU/CG
Sample : M3548-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VNJ-235

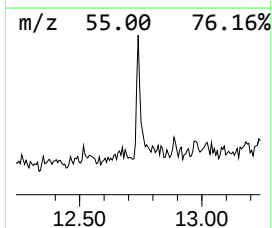
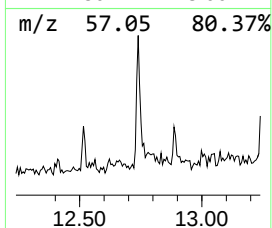
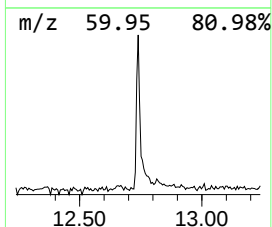
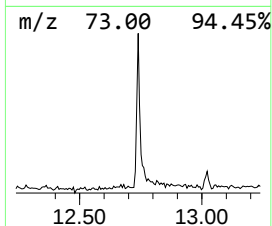
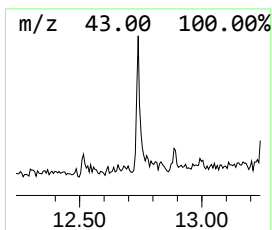
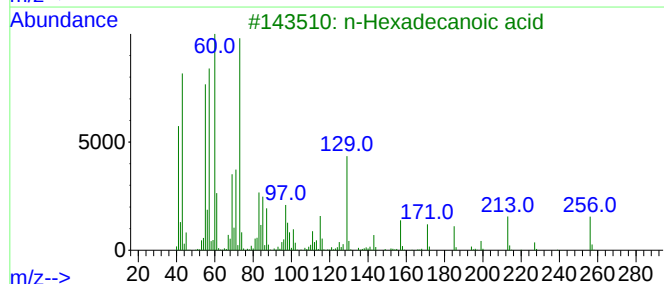
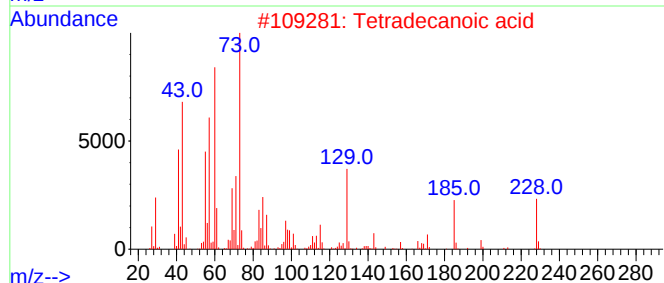
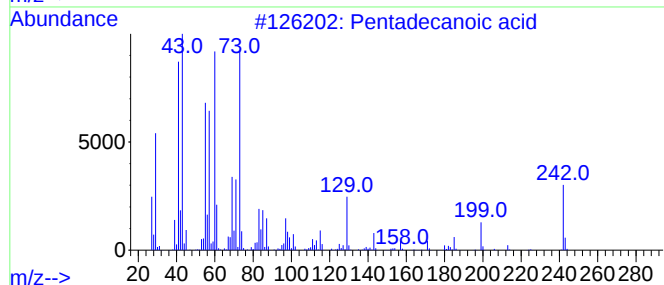
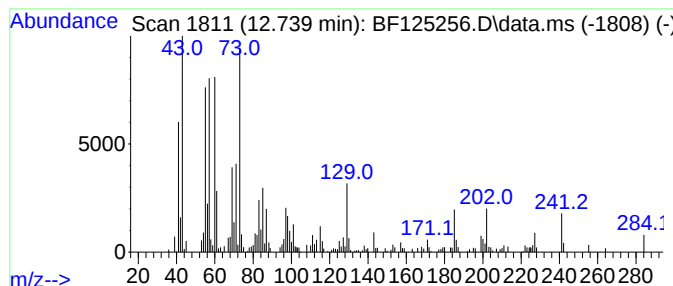
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Pentadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.739	2.71 ng	231820	Phenanthrene-d10	11.433

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecanoic acid	242	C15H30O2	001002-84-2	94
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	83
3			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	74
4			Dodecanoic acid	200	C12H24O2	000143-07-7	68
5			Undecanoic acid	186	C11H22O2	000112-37-8	58



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082721\
Data File : BF125256.D
Acq On : 27 Aug 2021 16:25
Operator : JU/CG
Sample : M3548-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VNJ-235

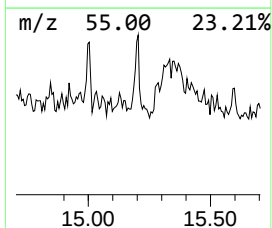
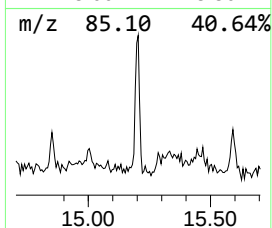
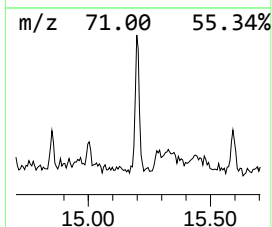
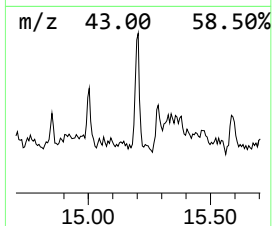
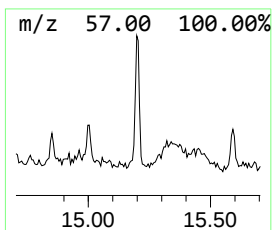
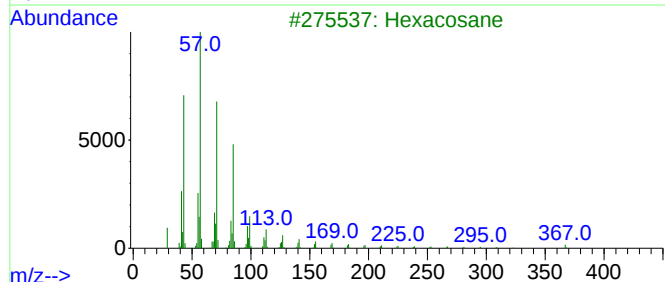
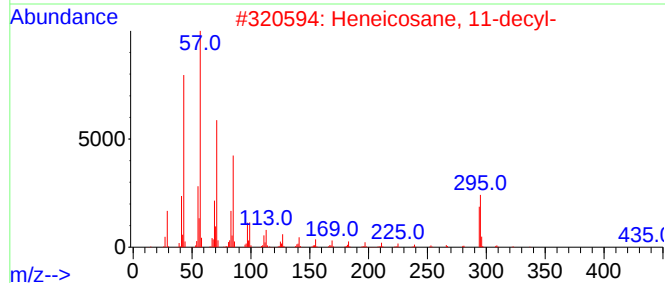
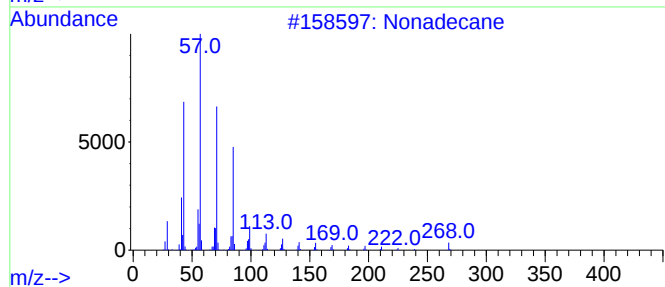
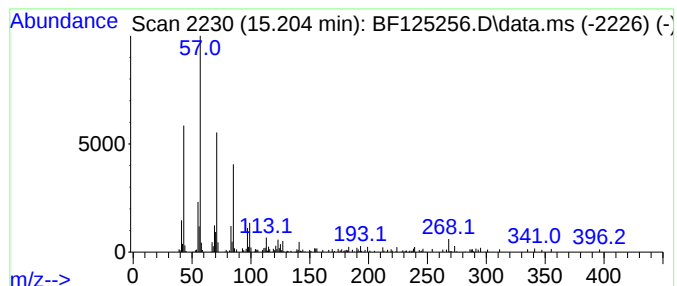
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Nonadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.204	2.63 ng	169200	Perylene-d12	15.574

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonadecane	268	C19H40	000629-92-5	91
2			Heneicosane, 11-decyl-	437	C31H64	055320-06-4	80
3			Hexacosane	366	C26H54	000630-01-3	80
4			Hentriacontane	437	C31H64	000630-04-6	80
5			Pentadecane	212	C15H32	000629-62-9	74



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082721\
Data File : BF125256.D
Acq On : 27 Aug 2021 16:25
Operator : JU/CG
Sample : M3548-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampled :
VNJ-235

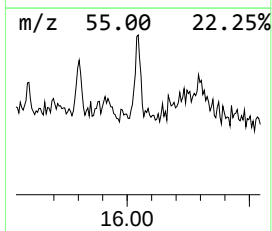
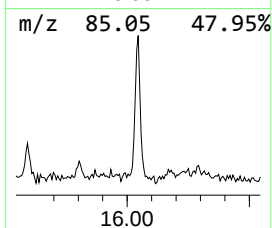
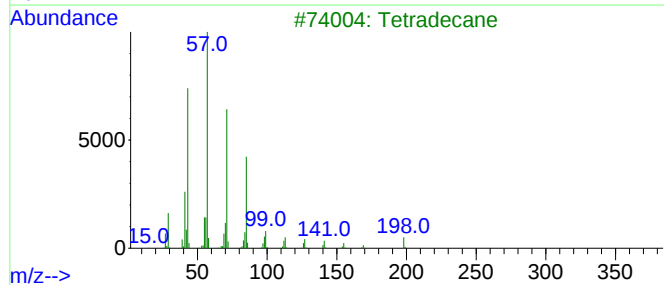
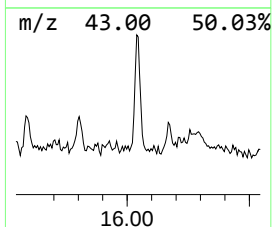
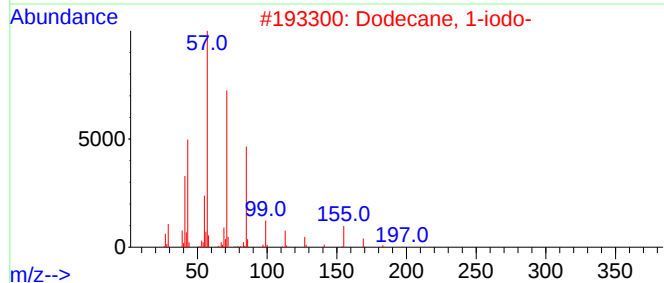
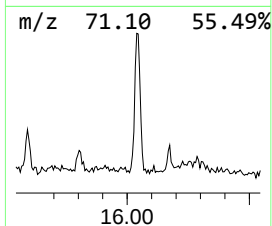
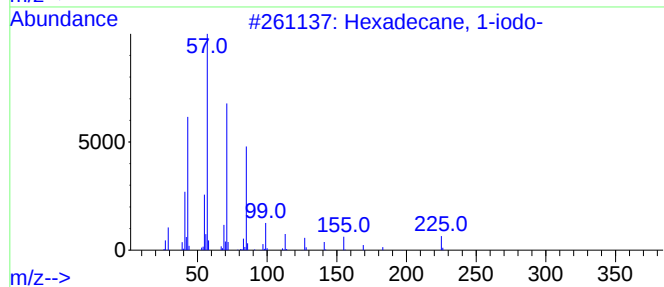
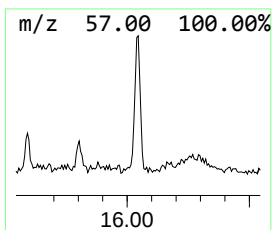
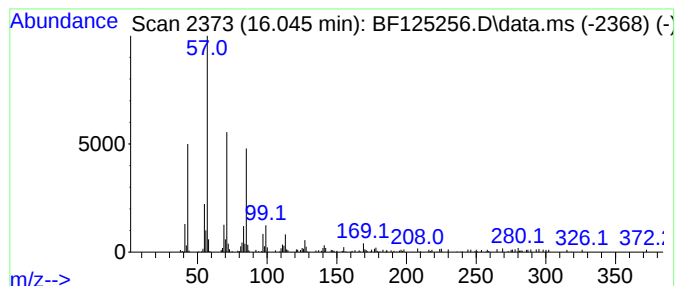
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Hexadecane, 1-iodo- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.045	3.28 ng	210818	Perylene-d12	15.574

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Hexadecane, 1-iodo-	352	C16H33I	000544-77-4	83
2		Dodecane, 1-iodo-	296	C12H25I	004292-19-7	83
3		Tetradecane	198	C14H30	000629-59-4	83
4		Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	80
5		Dotriacontane, 1-iodo-	576	C32H65I	1000406-32-4	80



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082721\
Data File : BF125256.D
Acq On : 27 Aug 2021 16:25
Operator : JU/CG
Sample : M3548-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VNJ-235

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.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
Butane, 2-metho...	2.199	26.5	ng	1498380	1	6.910	1131460	20.0
Ethylene glycol...	8.104	2.2	ng	162362	2	8.192	1450110	20.0
n-Hexadecanoic ...	11.951	6.5	ng	552366	4	11.433	1710150	20.0
Pentadecanoic acid	12.739	2.7	ng	231820	4	11.433	1710150	20.0
Nonadecane	15.204	2.6	ng	169200	6	15.574	1284640	20.0
Hexadecane, 1-i...	16.045	3.3	ng	210818	6	15.574	1284640	20.0