LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082321\
Data File : BF125164.D
Acq On : 23 Aug 2021 20:13
Operator : JU/CG
Sample : M3467-05
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SAMPLE-9-(322.00)

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: BF125164.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.234	18	25	34	rVB	1289582	1674085	41.59%	4.912%
2	5.157	515	522	527	rVB	61266	84032	2.09%	0.247%
3	5.539	582	587	590	rBV	3955099	3895856	96.78%	11.431%
4	6.539	751	757	760	rBV	3683523	4025623	100.00%	11.812%
5	6.922	818	822	825	rBV	1107796	928543	23.07%	2.724%
6	7.481	912	917	920	rBV	2728052	2629674	65.32%	7.716%
7	8.098	1019	1022	1036	rBV	183478	228944	5.69%	0.672%
8	8.204	1036	1040	1043	rBV	1473471	1208096	30.01%	3.545%
9	9.280	1218	1223	1226	rBV	4606201	4015524	99.75%	11.782%
10	9.957	1334	1338	1342	rBV	1600942	1366176	33.94%	4.009%
11	10.745	1468	1472	1476	rBV	3019364	2968827	73.75%	8.711%
12	11.445	1588	1591	1594	rBV	1675194	1433974	35.62%	4.207%
13	11.469	1594	1595	1598	rVB	101195	58993	1.47%	0.173%
14	11.963	1676	1679	1684	rBV	466058	414792	10.30%	1.217%
15	12.657	1794	1797	1801	rBV	408916	368209	9.15%	1.080%
16	12.751	1810	1813	1817	rBV2	149791	144513	3.59%	0.424%
17	12.886	1830	1836	1842	rVB	344144	351469	8.73%	1.031%
18	13.033	1857	1861	1864	rBV	3935951	3524510	87.55%	10.341%
19	13.104	1868	1873	1877	rBV3	29791	44267	1.10%	0.130%
20	13.198	1885	1889	1895	rVB4	33341	75870	1.88%	0.223%
21	13.315	1905	1909	1913	rBV2	40677	45324	1.13%	0.133%
22	13.721	1973	1978	1984	rBV	68136	73110	1.82%	0.215%
23	13.833	1993	1997	2000	rBV2	43492	56253	1.40%	0.165%
24	13.886	2004	2006	2010	rVB3	47590	48705	1.21%	0.143%
25	13.933	2010	2014	2015	rBV2	73466	81747	2.03%	0.240%
26	14.086	2032	2040	2043	rBV	1103717	1232637	30.62%	3.617%
27	14.110	2043	2044	2051	rVB	229124	189115	4.70%	0.555%
28	14.474	2103	2106	2109	rVB2	50349	48114	1.20%	0.141%
29	14.509	2109	2112	2116	rVB2	56714	49016	1.22%	0.144%
30	14.551	2116	2119	2121	rBV3	42523	50527	1.26%	0.148%
31	14.957	2183	2188	2194	rBV4	40237	73499	1.83%	0.216%
32	15.145	2215	2220	2223	rBV	318977	500133	12.42%	1.467%
33	15.221	2228	2233	2236	rBV2	109955	147736	3.67%	0.433%
34	15.456	2269	2273	2279	rVB	210098	265573	6.60%	0.779%
35	15.521	2280	2284	2290	rVB	135426	173991	4.32%	0.511%
36	15.586	2290	2295	2299	rBV	748165	1007368	25.02%	2.956%

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082321\
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Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SAMPLE-9-(322.00)

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

37	16.068	2374	2377	2382	rVB	60760	87146	2.16%	0.256%
38	16.139	2384	2389	2396	rBV10	45139	142353	3.54%	0.418%
39	16.903	2513	2519	2522	rBV6	32321	65915	1.64%	0.193%
40	17.092	2546	2551	2558	rBV3	83618	156682	3.89%	0.460%
41	17.550	2623	2629	2637	rVB2	70333	144846	3.60%	0.425%

Sum of corrected areas: 34081767

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082321\
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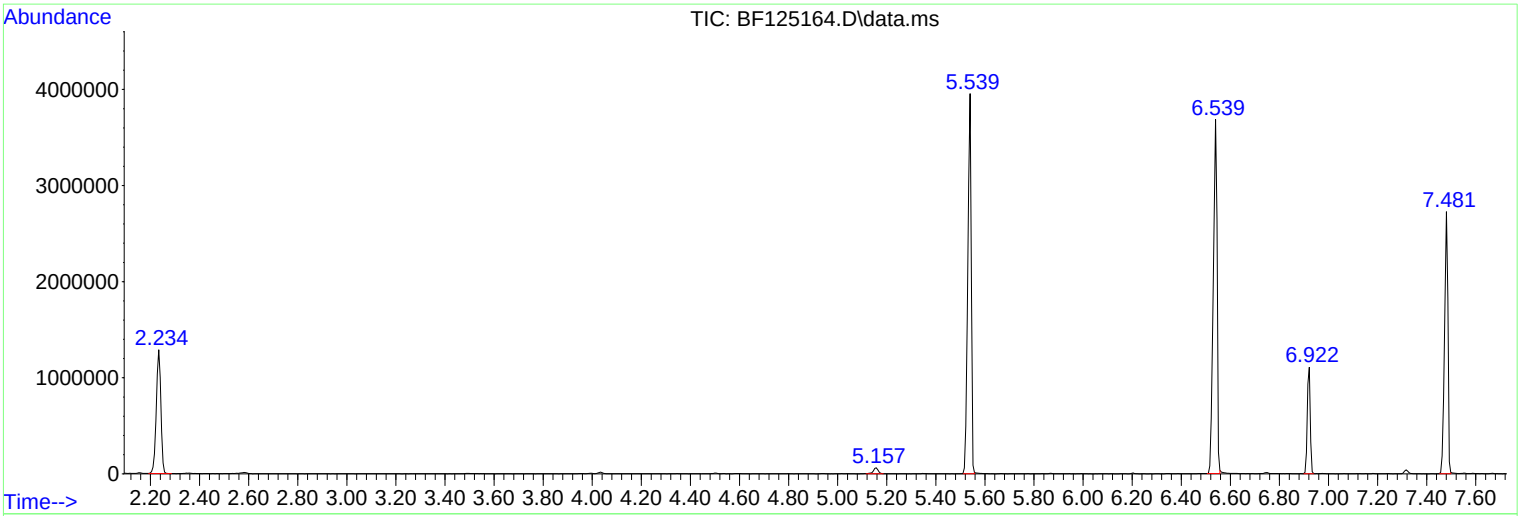
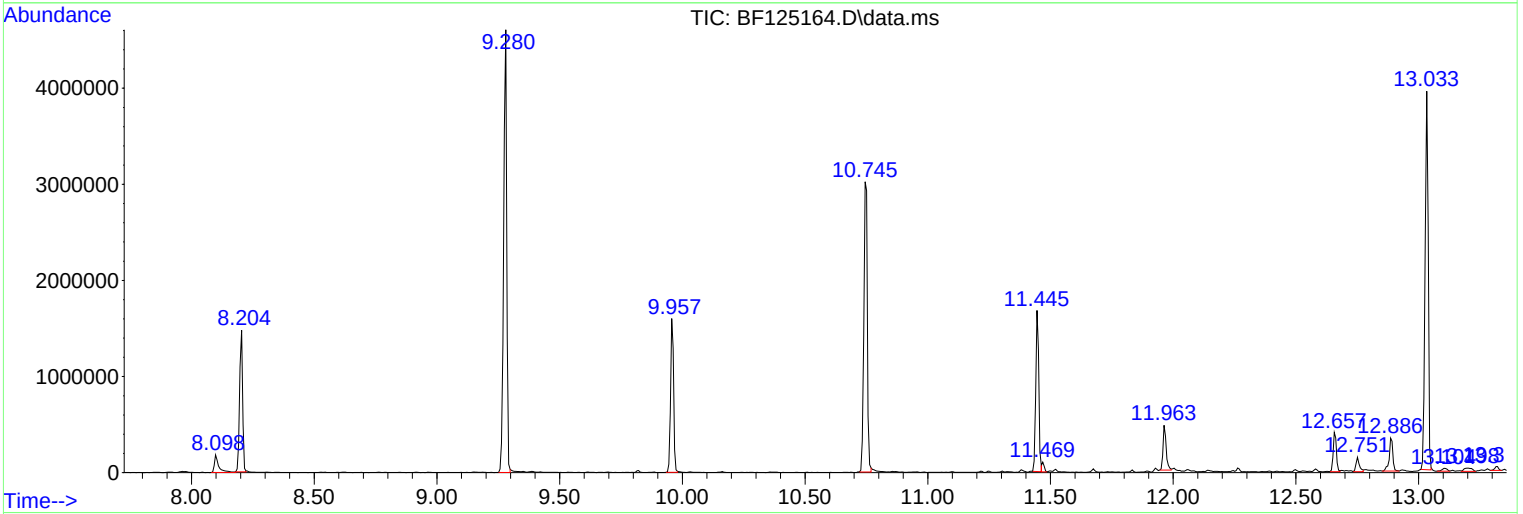
Misc :
ALS Vial : 8 Sample Multiplier: 1

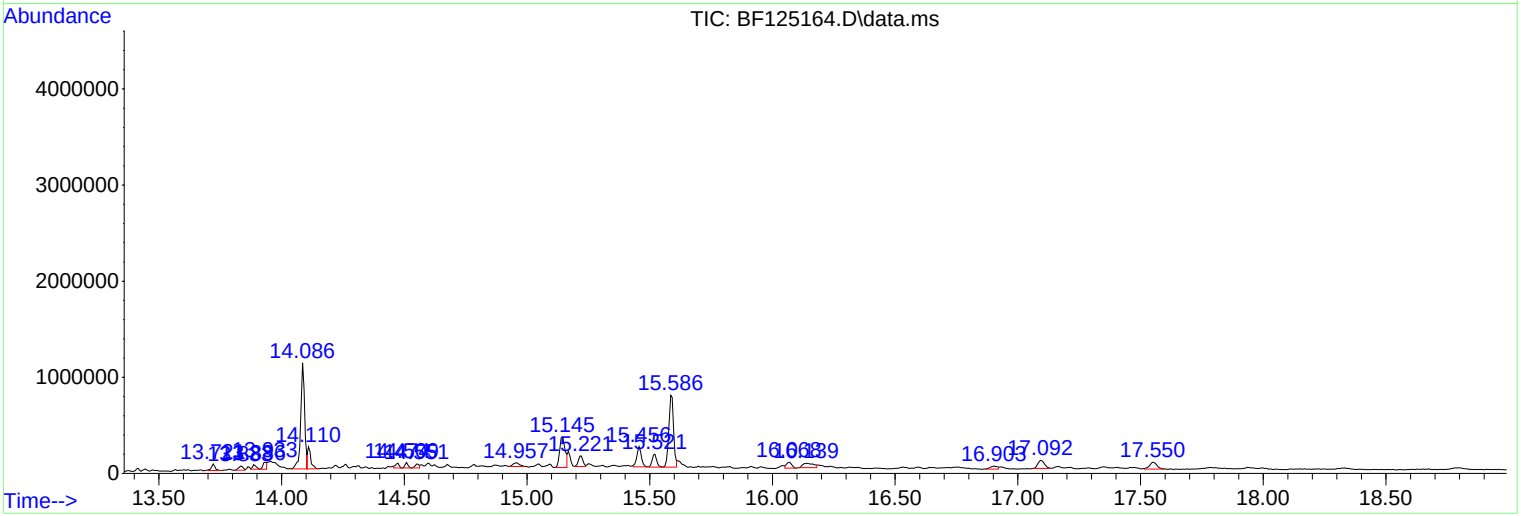
Instrument :
BNA_F
ClientSampleId :
SAMPLE-9-(322.00)

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







Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082321\
Data File : BF125164.D
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Operator : JU/CG
Sample : M3467-05
Misc :
ALS Vial : 8 Sample Multiplier: 1

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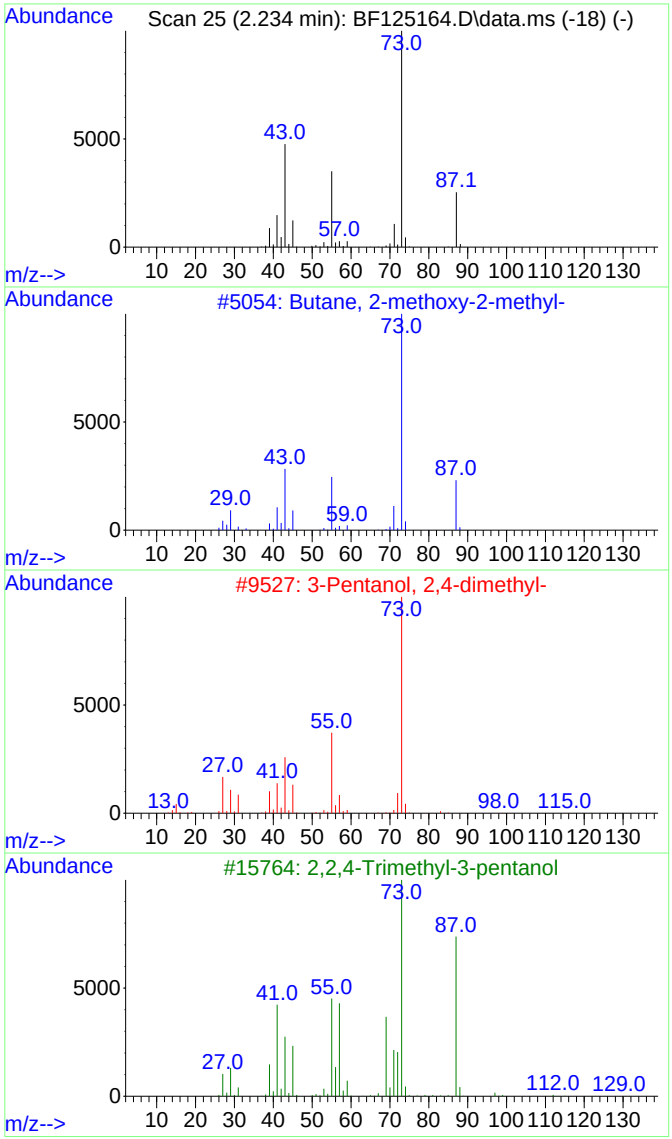
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

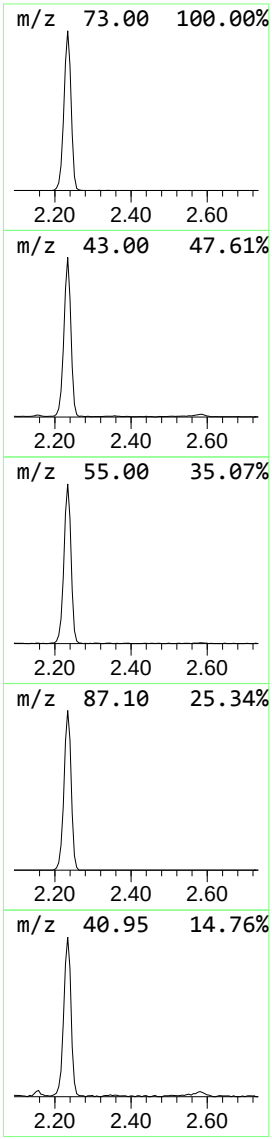
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.234	36.06 ng	1674090	1,4-Dichlorobenzene-d4	6.922

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	43
3	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
4	Silane, tetramethyl-	88	C4H12Si	000075-76-3	38
5	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	37





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Acq On : 23 Aug 2021 20:13
Operator : JU/CG
Sample : M3467-05
Misc :
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Instrument : BNA_F
ClientSampleId : SAMPLE-9-(322.00)

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

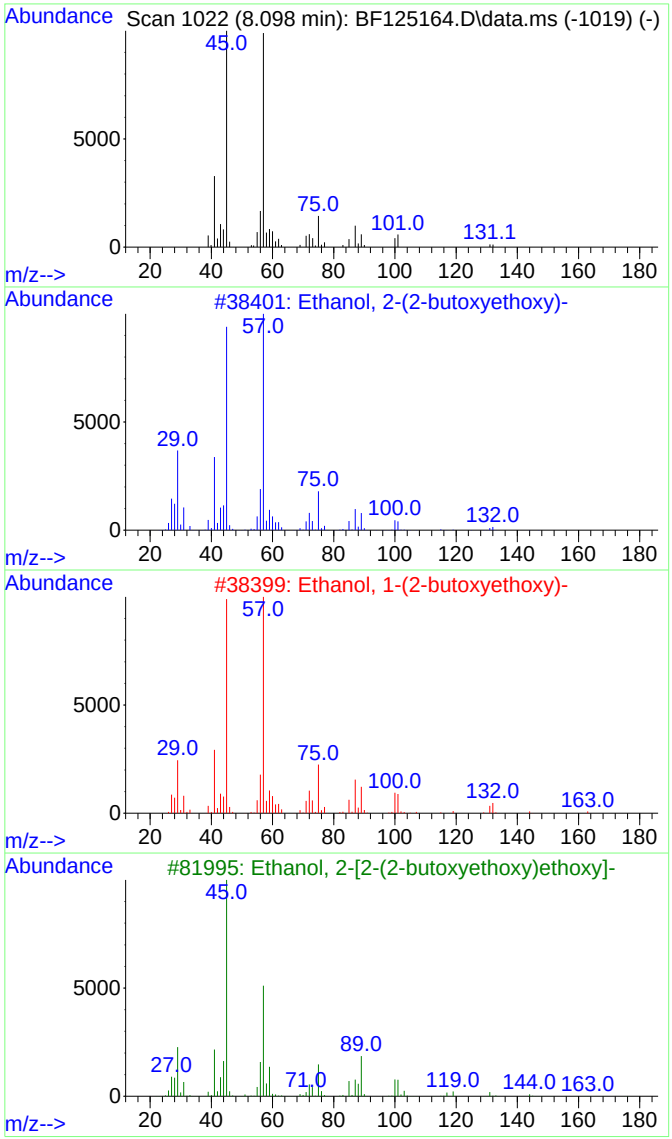
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

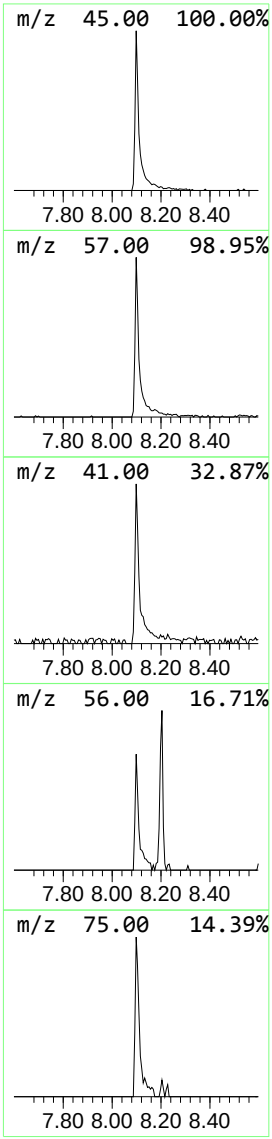
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.098	3.79 ng	228944	Naphthalene-d8	8.204

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-butoxyethoxy)et...	206	C10H22O4	000143-22-6	50
4	Butyl lactate	146	C7H14O3	000138-22-7	50
5	Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	50





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082321\
Data File : BF125164.D
Acq On : 23 Aug 2021 20:13
Operator : JU/CG
Sample : M3467-05
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SAMPLE-9-(322.00)

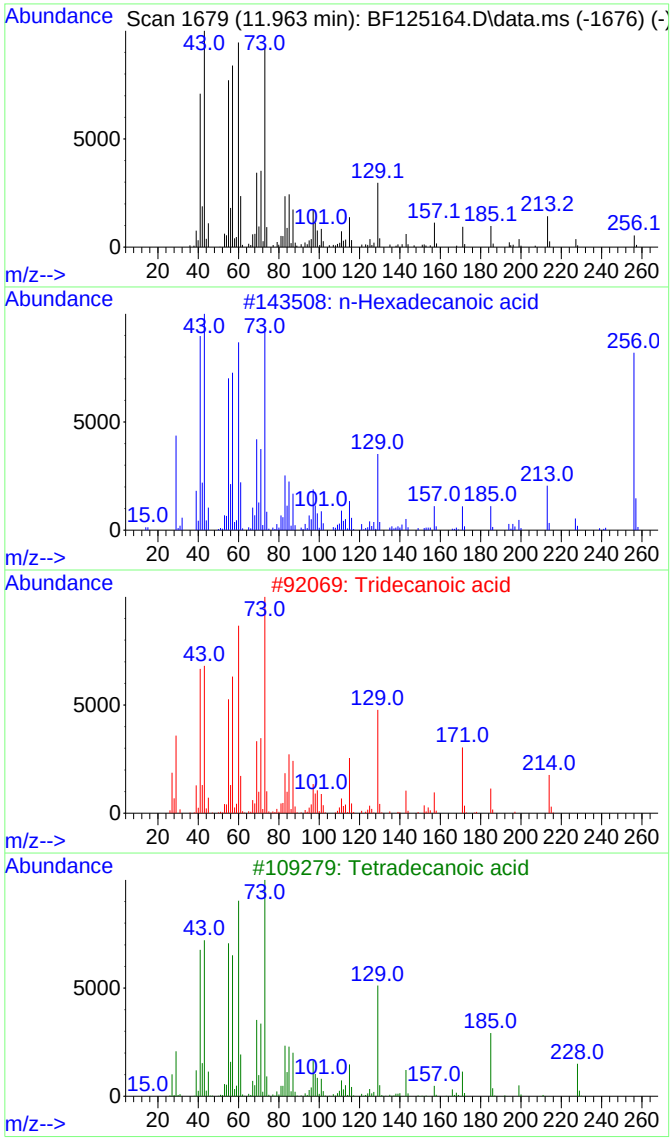
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

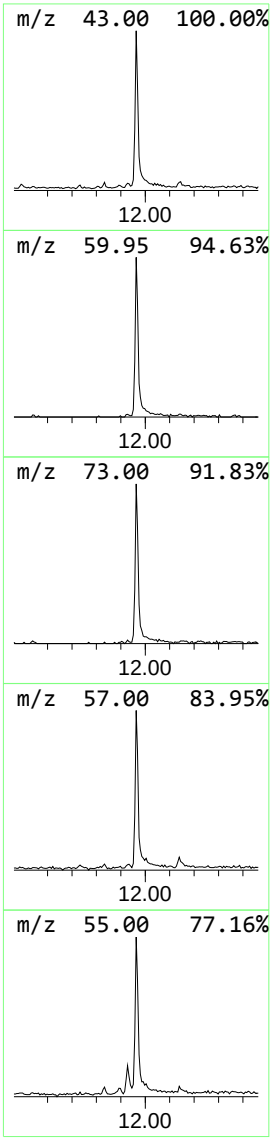
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.963	5.79 ng	414792	Phenanthrene-d10	11.445

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tridecanoic acid	214	C13H26O2	000638-53-9	95
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	86
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	83
5	Undecanoic acid	186	C11H22O2	000112-37-8	62





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082321\
Data File : BF125164.D
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Operator : JU/CG
Sample : M3467-05
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SAMPLE-9-(322.00)

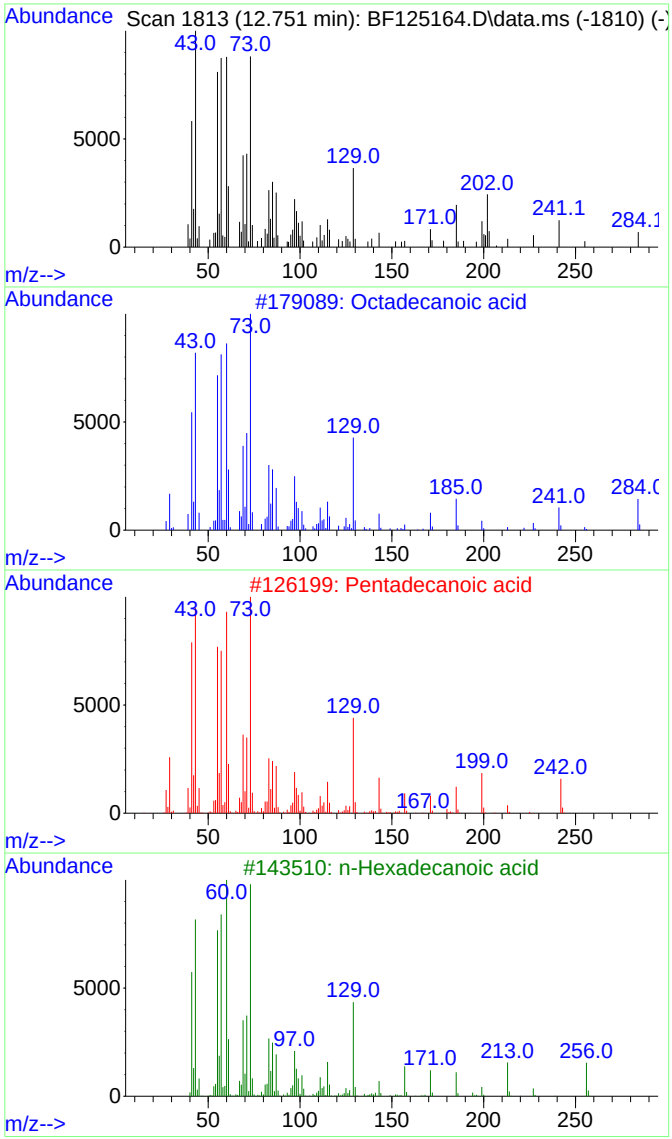
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

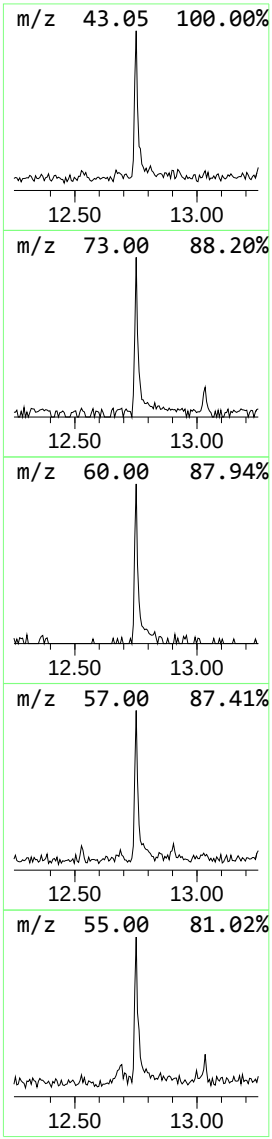
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Octadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.751	2.02 ng	144513	Phenanthrene-d10	11.445

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	87
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	83
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	72
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5	n-Decanoic acid	172	C10H20O2	000334-48-5	58





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082321\
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Misc :
ALS Vial : 8 Sample Multiplier: 1

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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
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TIC Library : C:\Database\NIST20.L
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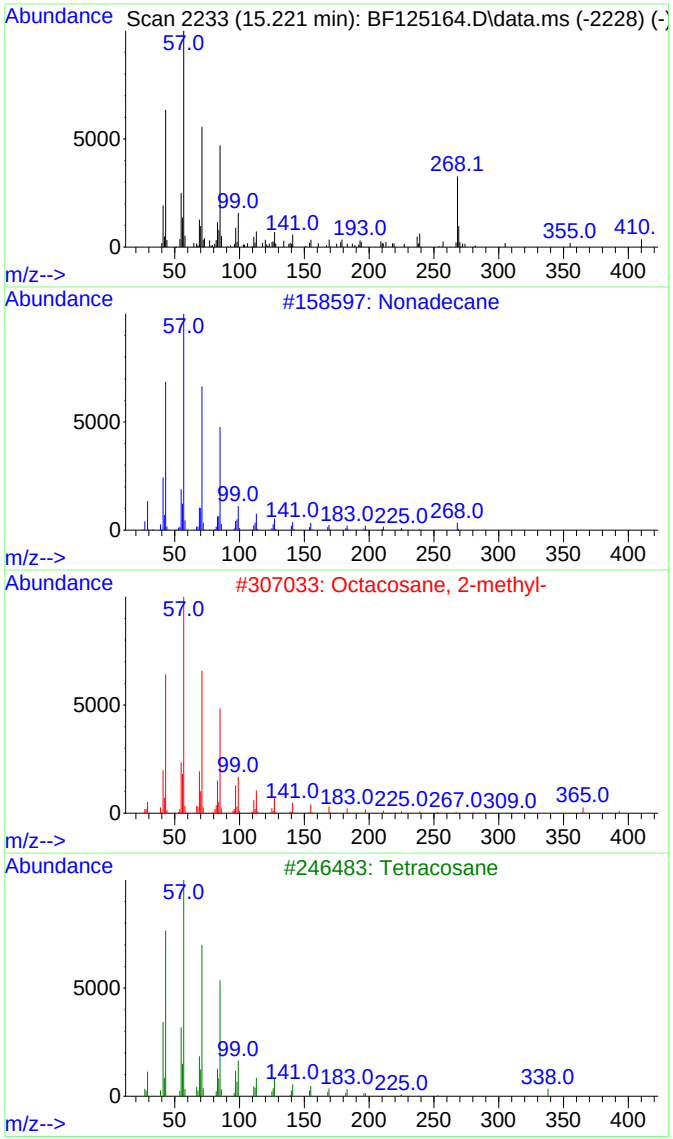
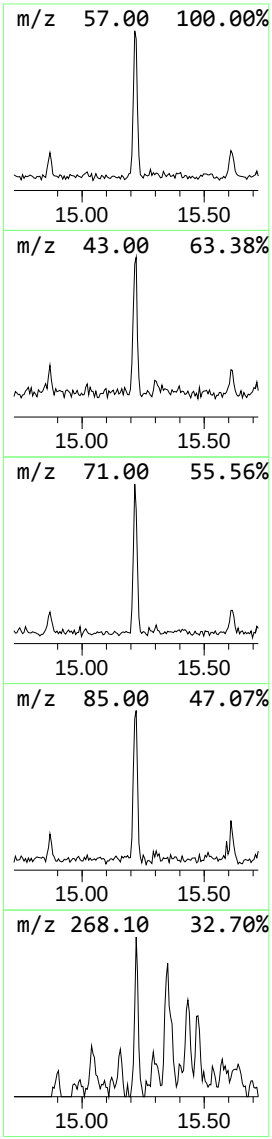
****

Peak Number 5 Nonadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.221	2.93 ng	147736	Perylene-d12	15.592

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane	268	C19H40	000629-92-5	81
2	Octacosane, 2-methyl-	408	C29H60	001560-98-1	70
3	Tetracosane	338	C24H50	000646-31-1	70
4	1-Iodoundecane	282	C11H23I	004282-44-4	70
5	Octacosane	394	C28H58	000630-02-4	70





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Data File : BF125164.D
Acq On : 23 Aug 2021 20:13
Operator : JU/CG
Sample : M3467-05
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SAMPLE-9-(322.00)

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

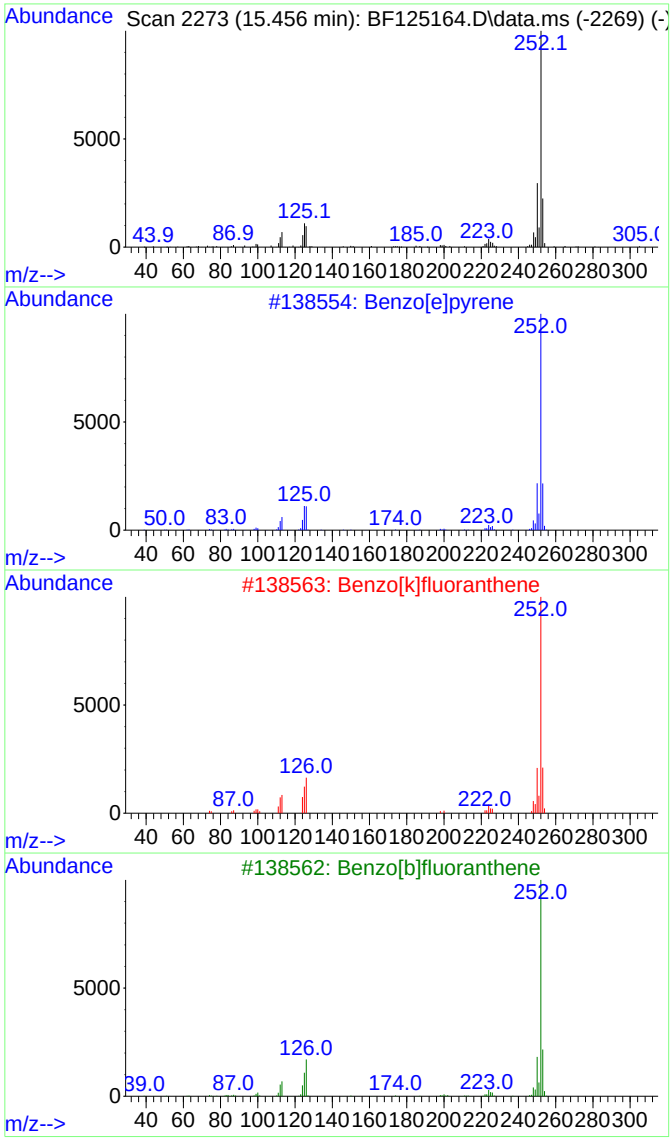
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

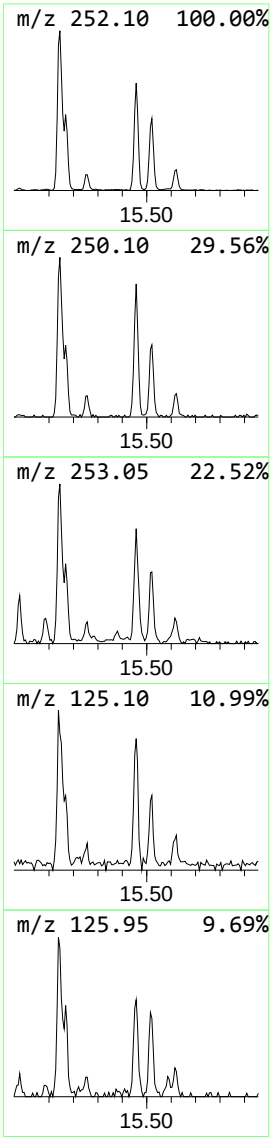
****

Peak Number 6 Benzo[e]pyrene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.457	5.27 ng	265573	Perylene-d12	15.592

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	99
2	Benzo[k]fluoranthene	252	C20H12	000207-08-9	98
3	Benzo[b]fluoranthene	252	C20H12	000205-99-2	95
4	Perylene	252	C20H12	000198-55-0	94
5	Benzo[j]fluoranthene	252	C20H12	000205-82-3	93





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Misc :
ALS Vial : 8 Sample Multiplier: 1

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ClientSampleId :
SAMPLE-9-(322.00)

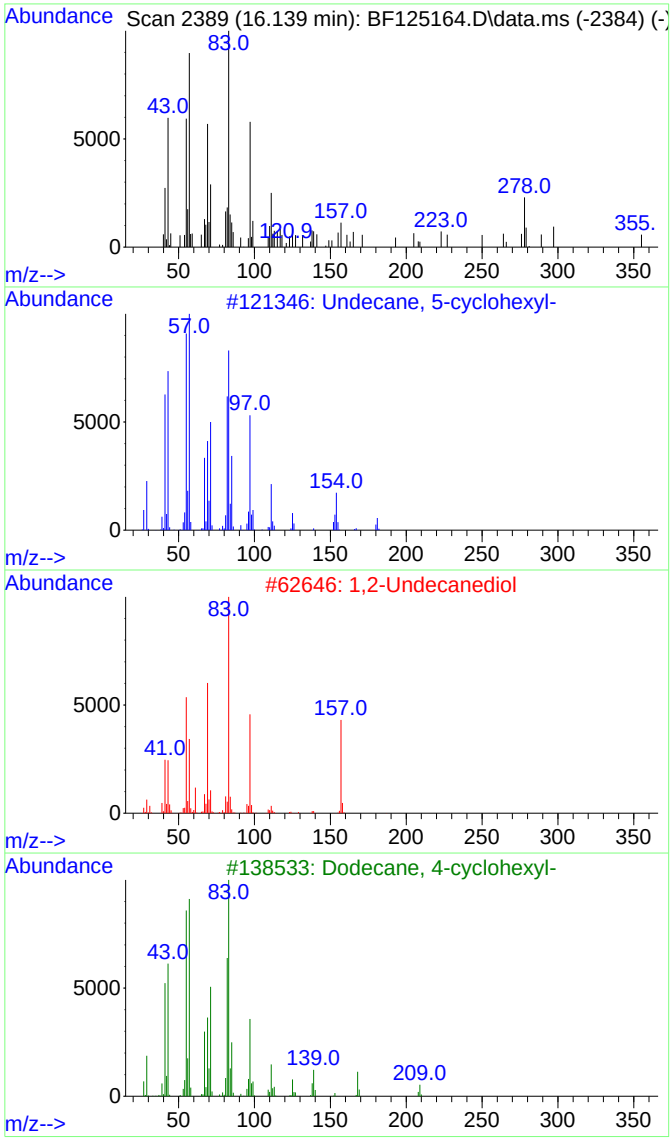
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

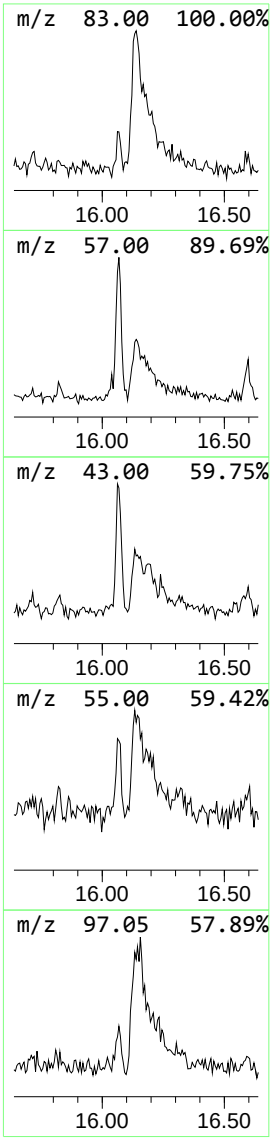
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Undecane, 5-cyclohexyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.139	2.83 ng	142353	Perylene-d12	15.592

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecane, 5-cyclohexyl-	238	C17H34	013151-80-9	53
2	1,2-Undecanediol	188	C11H24O2	013006-29-6	47
3	Dodecane, 4-cyclohexyl-	252	C18H36	013151-84-3	43
4	Binapacryl	322	C15H18N2O6	000485-31-4	35
5	Cyclohexane, 1,2-dimethyl-3-pent...	224	C16H32	062376-17-4	35





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082321\
Data File : BF125164.D
Acq On : 23 Aug 2021 20:13
Operator : JU/CG
Sample : M3467-05
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SAMPLE-9-(322.00)

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-metho...	2.234	36.1	ng	1674090	1	6.922	928543	20.0
Ethanol, 2-(2-b...	8.098	3.8	ng	228944	2	8.204	1208100	20.0
n-Hexadecanoic ...	11.963	5.8	ng	414792	4	11.445	1433970	20.0
Octadecanoic acid	12.751	2.0	ng	144513	4	11.445	1433970	20.0
Nonadecane	15.221	2.9	ng	147736	6	15.592	1007370	20.0
Benzo[e]pyrene	15.457	5.3	ng	265573	6	15.592	1007370	20.0
Undecane, 5-cyc...	16.139	2.8	ng	142353	6	15.592	1007370	20.0