LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082225\
Data File : BF143566.D
Acq On : 22 Aug 2025 12:02
Operator : RC/JU
Sample : Q2903-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-6A-081925

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-BF082025.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF143566.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.257	3	11	22	rVB	2098025	3491038	83.69%	13.009%
2	5.157	495	504	511	rBV2	92917	170615	4.09%	0.636%
3	5.563	567	573	593	rBV	1240584	1649212	39.54%	6.145%
4	6.557	737	742	759	rBV	855583	1123617	26.94%	4.187%
5	6.922	799	804	812	rBV	527875	653934	15.68%	2.437%
6	7.487	889	900	905	rBV	1539004	2261353	54.21%	8.427%
7	7.957	972	980	998	rBV	11779	41790	1.00%	0.156%
8	8.098	999	1004	1013	rBV	120898	218252	5.23%	0.813%
9	8.204	1017	1022	1033	rVB	702802	899967	21.58%	3.354%
10	9.281	1199	1205	1210	rBV	2975849	3976214	95.32%	14.817%
11	9.963	1316	1321	1326	rBV	880098	1091060	26.16%	4.066%
12	10.675	1436	1442	1447	rBV	88785	122786	2.94%	0.458%
13	10.757	1450	1456	1471	rBV	2172493	2980554	71.45%	11.106%
14	11.116	1512	1517	1527	rBV	48252	80842	1.94%	0.301%
15	11.451	1568	1574	1588	rBV	925544	1241357	29.76%	4.626%
16	11.898	1646	1650	1657	rBV	66927	121744	2.92%	0.454%
17	11.974	1657	1663	1676	rVV2	350135	605432	14.51%	2.256%
18	12.516	1751	1755	1761	rBV5	18981	44927	1.08%	0.167%
19	12.680	1779	1783	1792	rBV2	68292	136596	3.27%	0.509%
20	12.763	1792	1797	1808	rVV	74957	151611	3.63%	0.565%
21	13.039	1838	1844	1849	rBV	3090788	4171254	100.00%	15.543%
22	14.098	2019	2024	2031	rVB	486616	648328	15.54%	2.416%
23	14.945	2163	2168	2178	rVB	252639	343883	8.24%	1.281%
24	15.592	2273	2278	2296	rVB	366081	609840	14.62%	2.272%

Sum of corrected areas: 26836206

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082225\
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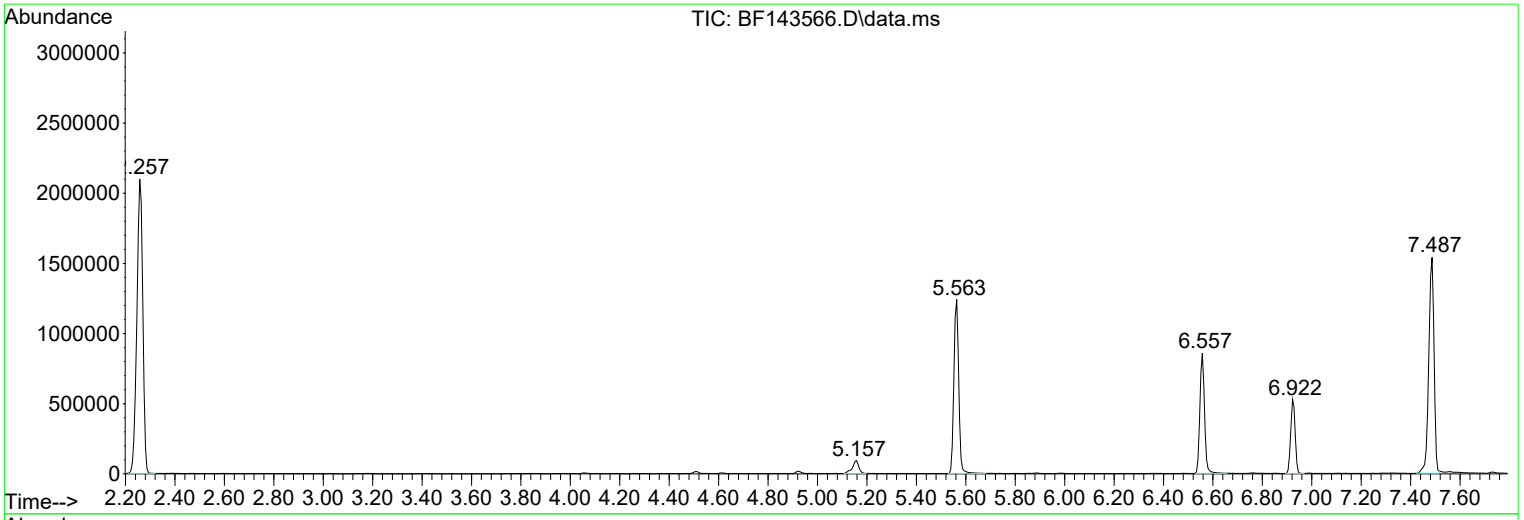
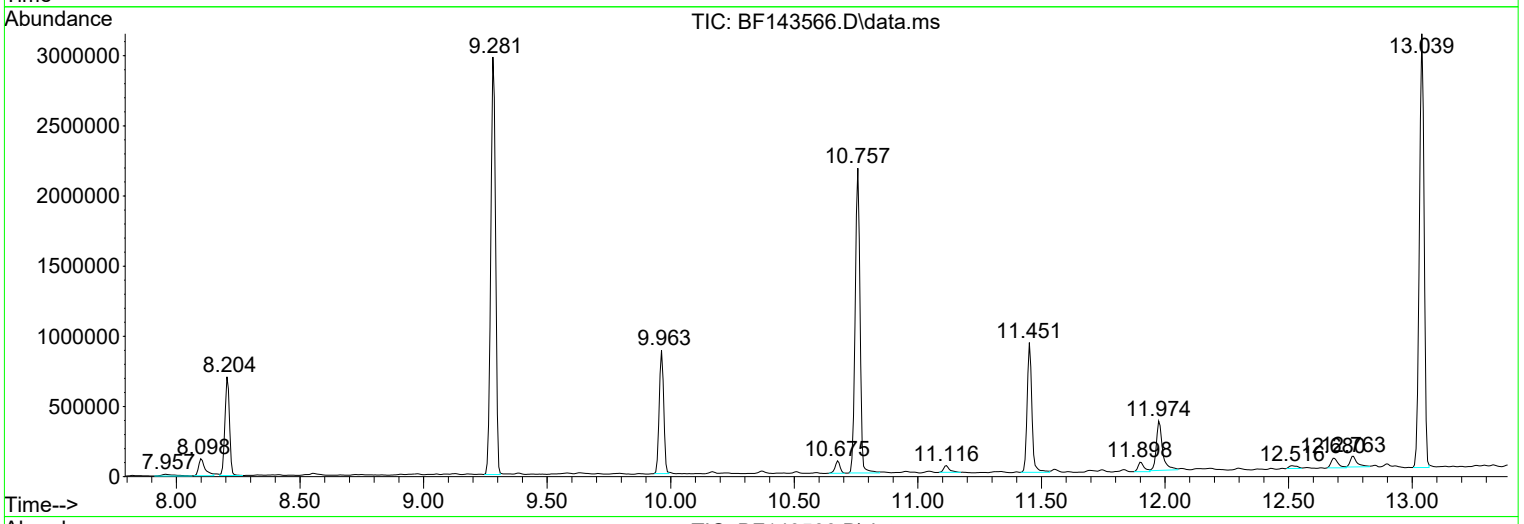
Operator : RC/JU
Sample : Q2903-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

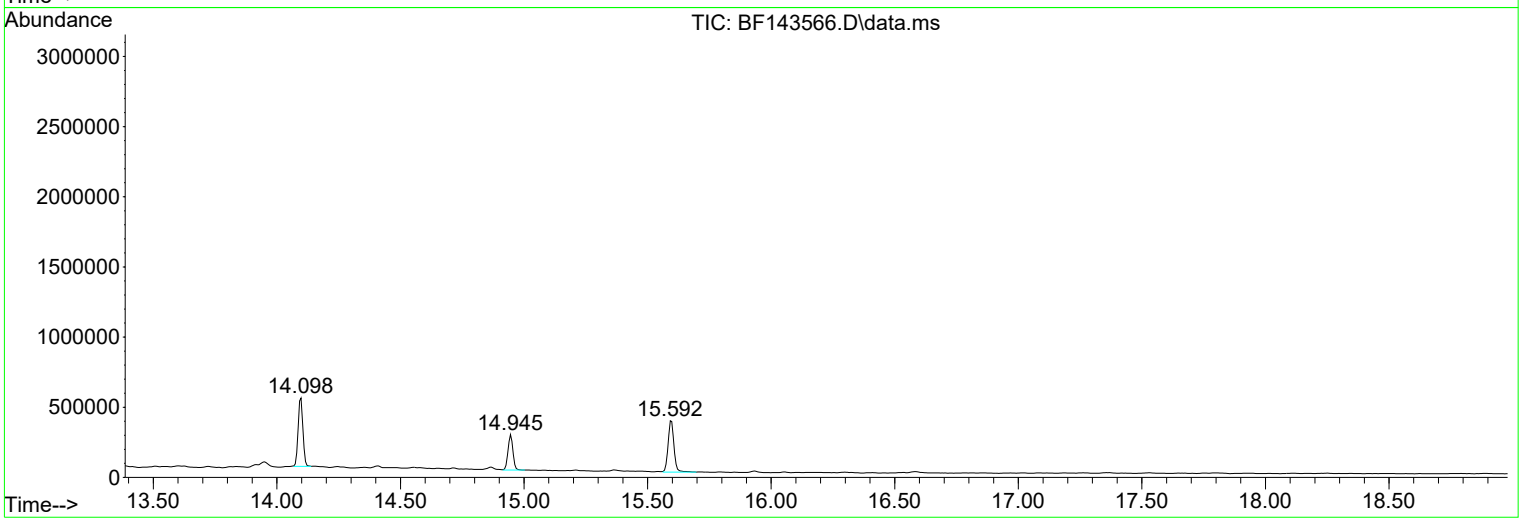
Instrument :
BNA_F
ClientSampleId :
MW-6A-081925

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082025.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 : BF143566.D
Acq On : 22 Aug 2025 12:02
Operator : RC/JU
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Misc :
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Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082025.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

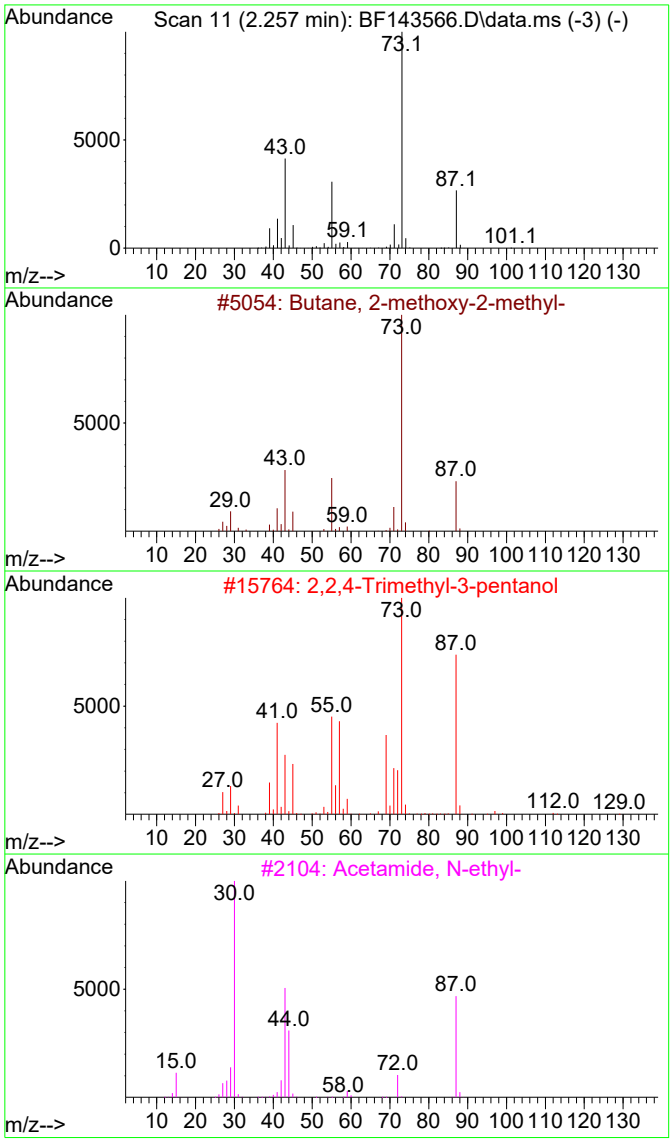
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

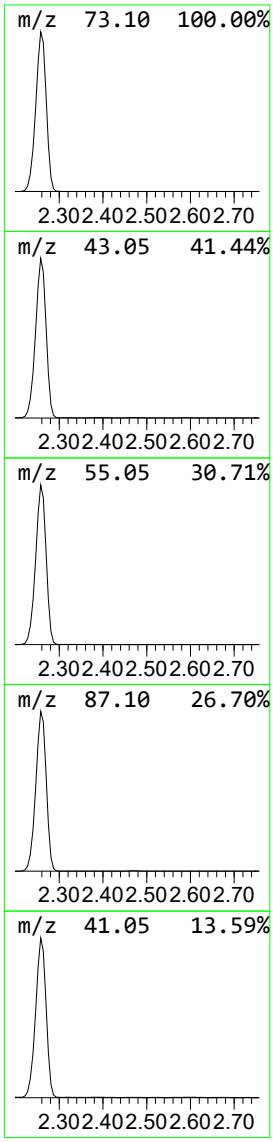
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.257	106.77 ng	3491040	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	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	27
4	Octanal, 7-methoxy-3,7-dimethyl-	186	C11H22O2	003613-30-7	17
5	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12





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Data File : BF143566.D
Acq On : 22 Aug 2025 12:02
Operator : RC/JU
Sample : Q2903-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-6A-081925

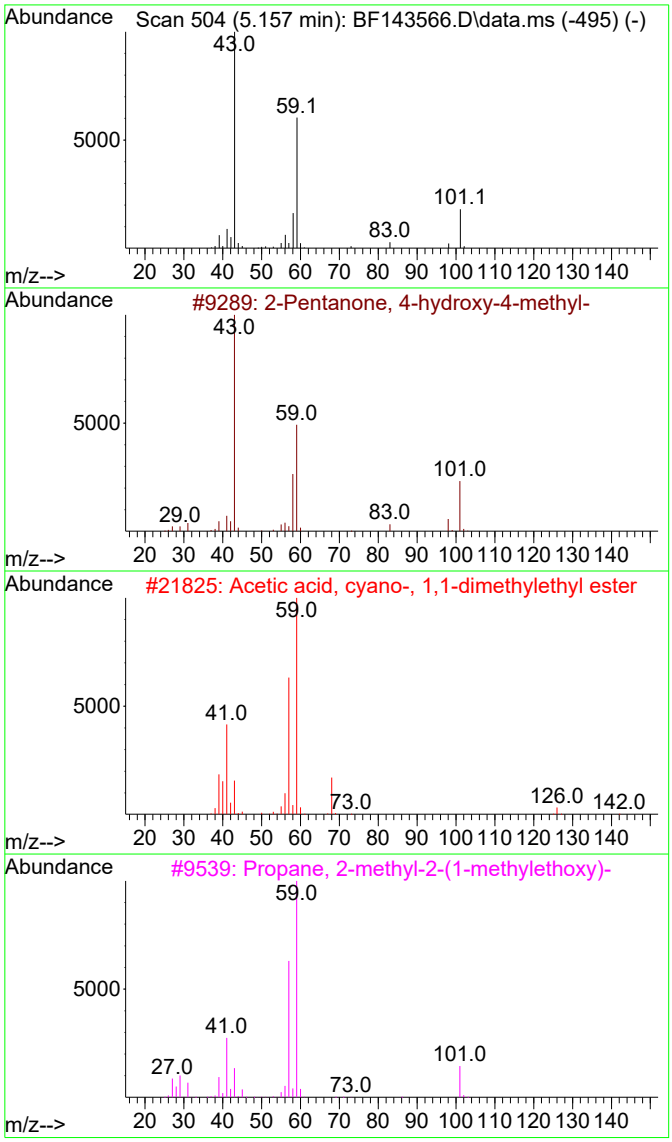
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082025.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

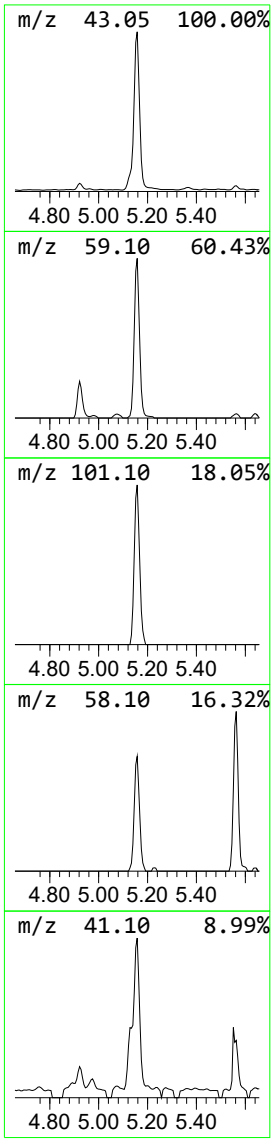
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.157	5.22 ng	170615	1,4-Dichlorobenzene-d4	6.922

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	37
3	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
5	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082225\
Data File : BF143566.D
Acq On : 22 Aug 2025 12:02
Operator : RC/JU
Sample : Q2903-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-6A-081925

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082025.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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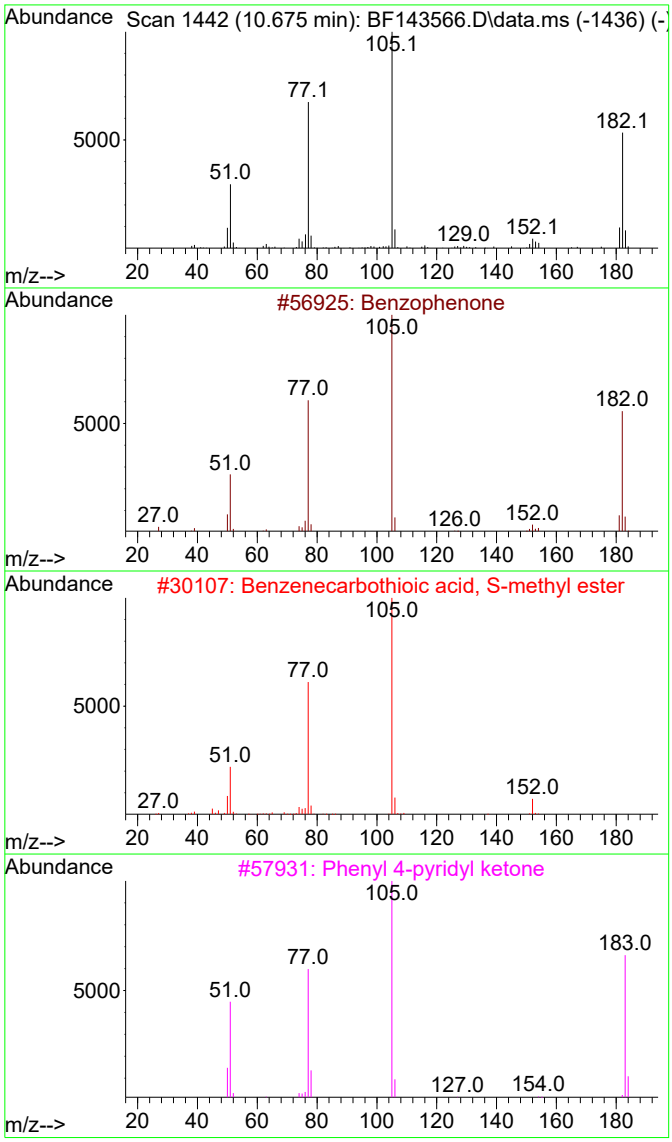
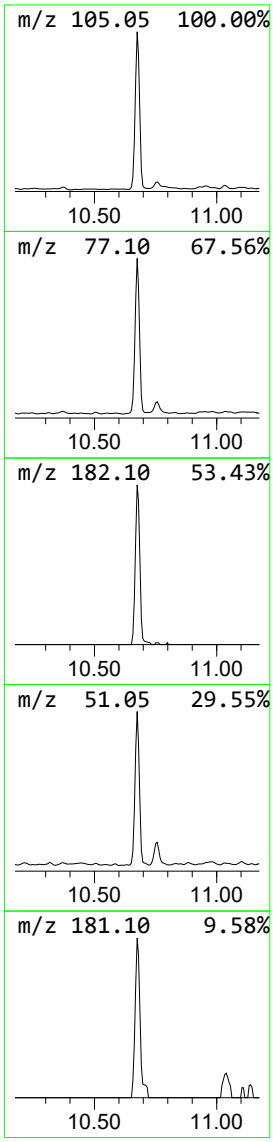
Peak Number 4 Benzophenone Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.675	2.25 ng	122786	Acenaphthene-d10	9.963

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	52
3	Phenyl 4-pyridyl ketone	183	C12H9NO	014548-46-0	50
4	Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	49
5	Ethanedione, diphenyl-	210	C14H10O2	000134-81-6	47





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082225\
Data File : BF143566.D
Acq On : 22 Aug 2025 12:02
Operator : RC/JU
Sample : Q2903-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-6A-081925

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082025.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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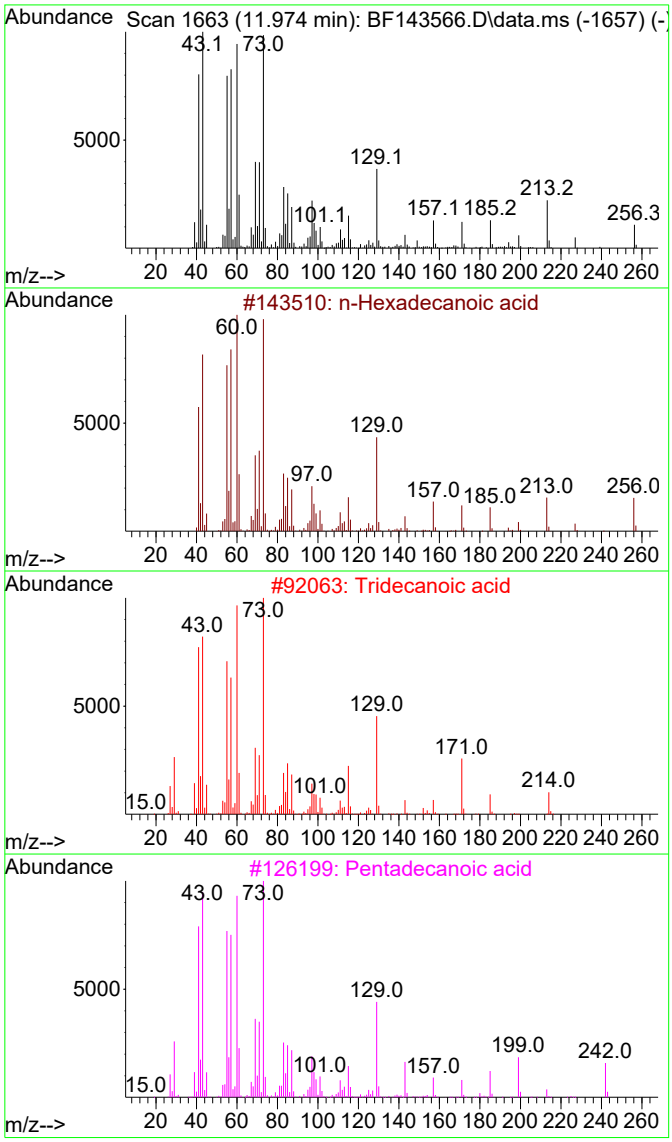
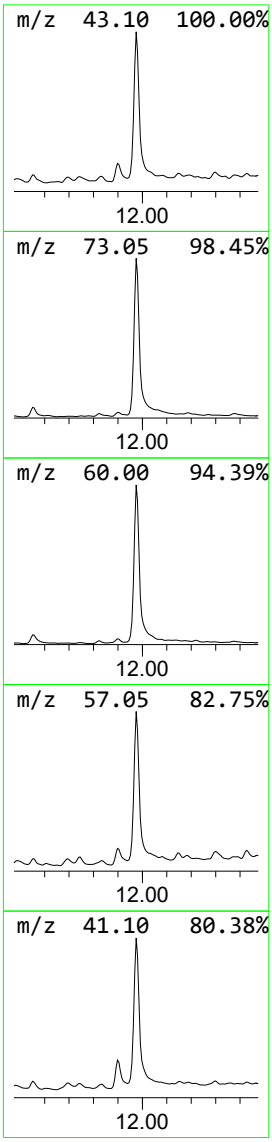
Peak Number 5 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.975	9.75 ng	605432	Phenanthrene-d10	11.451

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	94
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	74
5	Undecanoic acid	186	C11H22O2	000112-37-8	74





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082225\
Data File : BF143566.D
Acq On : 22 Aug 2025 12:02
Operator : RC/JU
Sample : Q2903-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-6A-081925

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082025.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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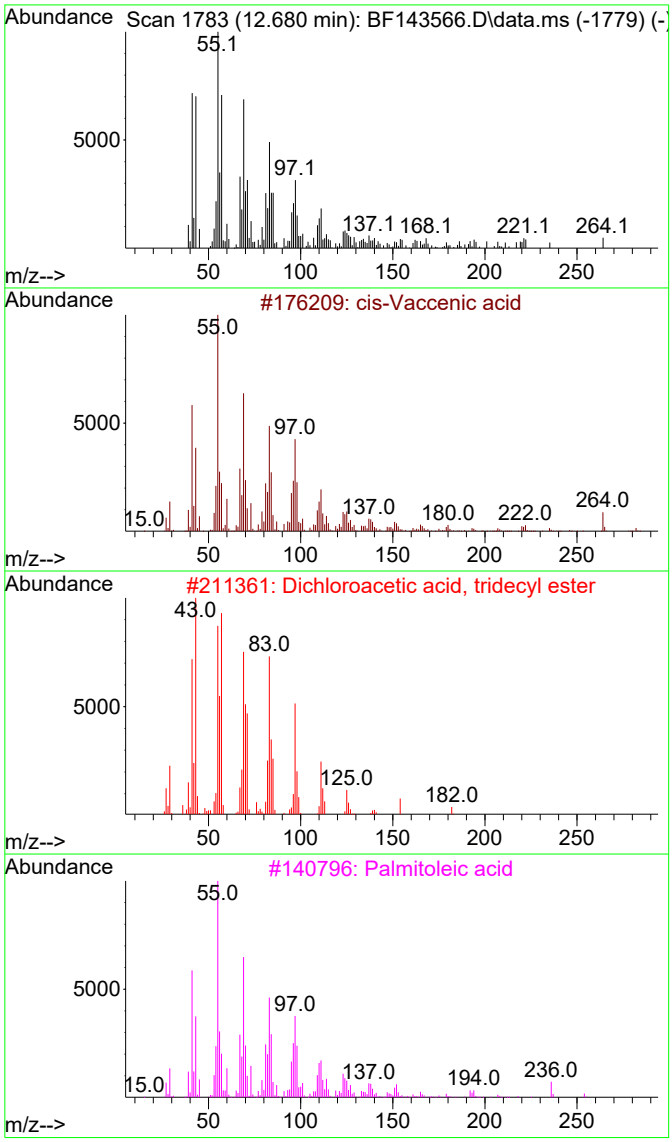
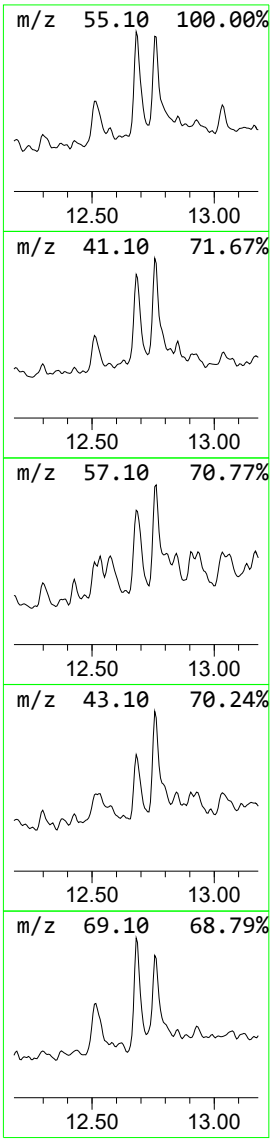
Peak Number 6 cis-Vaccenic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.680	2.20 ng	136596	Phenanthrene-d10	11.451

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	cis-Vaccenic acid	282	C18H34O2	000506-17-2	72
2	Dichloroacetic acid, tridecyl ester	310	C15H28Cl2O2	1000280-48-3	70
3	Palmitoleic acid	254	C16H30O2	000373-49-9	68
4	2- Chloropropionic acid, hexadec...	332	C19H37ClO2	086711-81-1	62
5	Dichloroacetic acid, tetradecyl ...	324	C16H30Cl2O2	083005-02-1	60





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082225\
Data File : BF143566.D
Acq On : 22 Aug 2025 12:02
Operator : RC/JU
Sample : Q2903-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-6A-081925

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082025.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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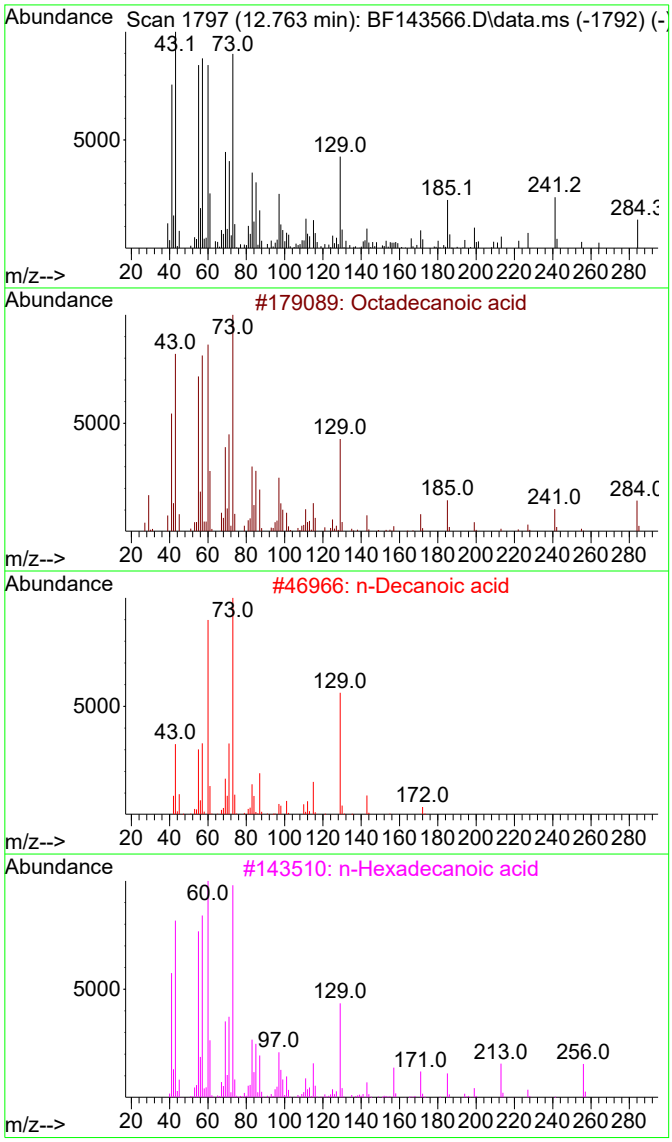
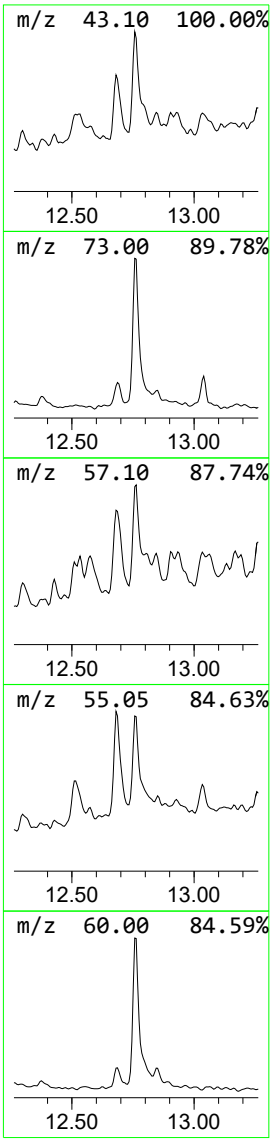
Peak Number 7 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.763	2.44 ng	151611	Phenanthrene-d10	11.451

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	n-Decanoic acid	172	C10H20O2	000334-48-5	90
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	83
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	83
5	Dodecanoic acid	200	C12H24O2	000143-07-7	68





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ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-6A-081925

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082025.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

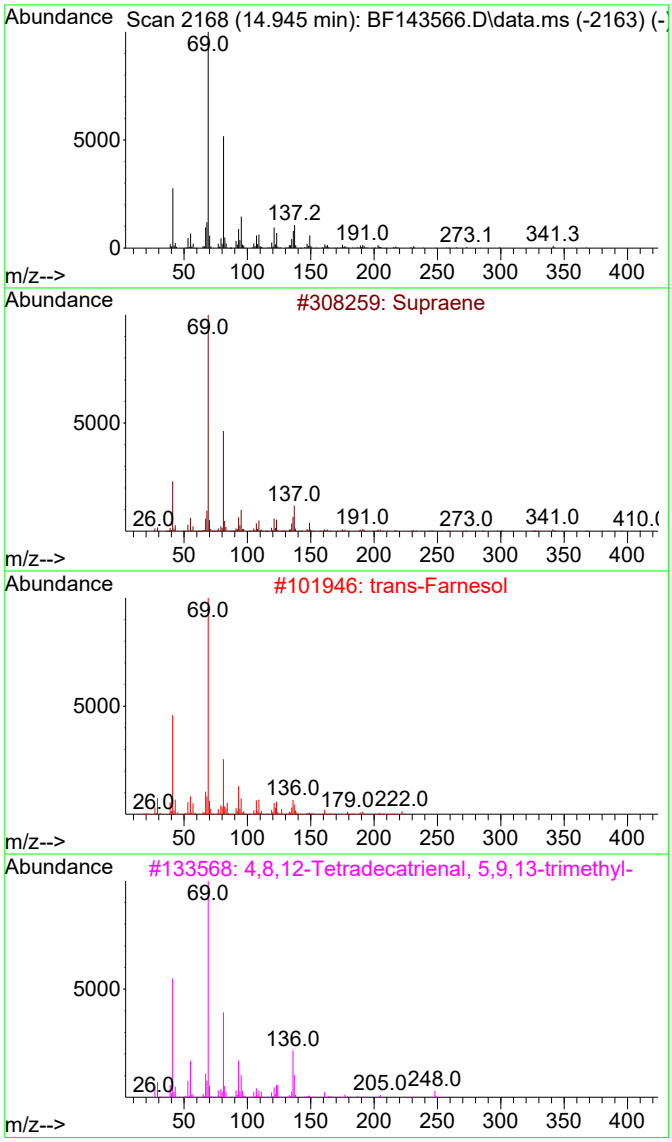
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

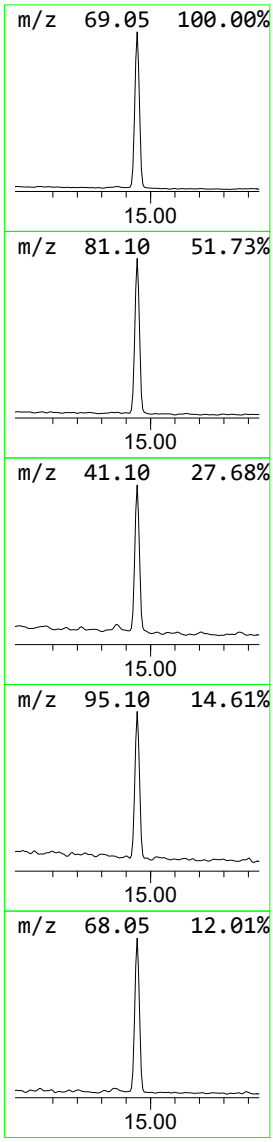
****

Peak Number 8 Supraene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.945	11.28 ng	343883	Perylene-d12	15.592

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Supraene	410	C30H50	007683-64-9	91
2	trans-Farnesol	222	C15H26O	000106-28-5	64
3	4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	64
4	3,7-Dimethyl-1-phenylsulfonyl-2,...	278	C16H22O2S	1000432-27-5	59
5	1,5-Heptadiene, 3,3,6-trimethyl-	138	C10H18	035387-63-4	52





Tentatively Identified Compound (LSC) summary

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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...	2.257	106.8	ng	3491040	1	6.922	653934	20.0
2-Pentanone, 4-...	5.157	5.2	ng	170615	1	6.922	653934	20.0
Benzophenone	10.675	2.3	ng	122786	3	9.963	1091060	20.0
n-Hexadecanoic ...	11.975	9.8	ng	605432	4	11.451	1241360	20.0
cis-Vaccenic acid	12.680	2.2	ng	136596	4	11.451	1241360	20.0
Octadecanoic acid	12.763	2.4	ng	151611	4	11.451	1241360	20.0
Supraene	14.945	11.3	ng	343883	6	15.592	609840	20.0