LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF053025\
Data File : BF142587.D
Acq On : 30 May 2025 23:41
Operator : RC/JU
Sample : Q2153-01
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TR-04-0592025

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-BF052025.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF142587.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.275	9	14	26	rVB	14615	26554	1.72%	0.183%
2	5.110	488	496	504	rBV	112017	160690	10.41%	1.106%
3	5.510	558	564	579	rBV	1181303	1544102	100.00%	10.624%
4	6.522	730	736	753	rVB	1117433	1512253	97.94%	10.405%
5	6.898	795	800	805	rBV	567075	686769	44.48%	4.725%
6	7.457	889	895	900	rBV	727407	910624	58.97%	6.266%
7	7.710	930	938	944	rVB4	10728	16225	1.05%	0.112%
8	8.181	1011	1018	1026	rBV	658797	827753	53.61%	5.695%
9	9.257	1195	1201	1206	rBV	1184795	1481461	95.94%	10.193%
10	9.334	1210	1214	1222	rVB2	14451	20816	1.35%	0.143%
11	9.522	1241	1246	1251	rBV	13016	21374	1.38%	0.147%
12	9.592	1251	1258	1261	rBV	15634	27734	1.80%	0.191%
13	9.651	1265	1268	1275	rVB5	12857	22682	1.47%	0.156%
14	9.798	1289	1293	1298	rBV	24438	33218	2.15%	0.229%
15	9.863	1299	1304	1309	rBV	16510	22004	1.43%	0.151%
16	9.939	1311	1317	1326	rVV	598664	774318	50.15%	5.328%
17	10.139	1347	1351	1355	rVB3	10870	16335	1.06%	0.112%
18	10.181	1355	1358	1363	rBV4	11844	15762	1.02%	0.108%
19	10.251	1367	1370	1373	rBV3	11827	17913	1.16%	0.123%
20	10.363	1382	1389	1393	rBV3	39628	60304	3.91%	0.415%
21	10.581	1422	1426	1432	rVB	24362	43014	2.79%	0.296%
22	10.651	1433	1438	1444	rVV	69582	101015	6.54%	0.695%
23	10.728	1445	1451	1461	rVV	639596	857140	55.51%	5.898%
24	10.839	1465	1470	1478	rVB	82105	148661	9.63%	1.023%
25	11.033	1499	1503	1505	rBV3	12474	19140	1.24%	0.132%
26	11.286	1541	1546	1549	rBV	75794	107117	6.94%	0.737%
27	11.316	1549	1551	1557	rVB2	44986	57417	3.72%	0.395%
28	11.428	1565	1570	1580	rBV2	547540	809606	52.43%	5.570%
29	11.663	1607	1610	1614	rBV2	14899	19730	1.28%	0.136%
30	11.716	1615	1619	1623	rVB	69587	86143	5.58%	0.593%
31	11.945	1652	1658	1666	rBV2	137155	247619	16.04%	1.704%
32	12.039	1671	1674	1682	rVB3	34712	70562	4.57%	0.486%
33	12.122	1684	1688	1692	rVV	63260	78219	5.07%	0.538%
34	12.480	1745	1749	1750	rBV2	29125	37182	2.41%	0.256%
35	12.516	1751	1755	1761	rVB2	99142	174065	11.27%	1.198%
36	12.639	1772	1776	1781	rBV	145784	187659	12.15%	1.291%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF053025\
Data File : BF142587.D
Acq On : 30 May 2025 23:41
Operator : RC/JU
Sample : Q2153-01
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TR-04-0592025

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-BF052025.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	12.733	1789	1792	1797	rBV2	29519	49063	3.18%	0.338%
38	12.869	1811	1815	1822	rBV	152507	245197	15.88%	1.687%
39	13.010	1834	1839	1847	rVB	1093981	1406345	91.08%	9.676%
40	14.069	2014	2019	2026	rBV2	618140	1009419	65.37%	6.945%
41	15.568	2270	2274	2284	rVB	327657	580639	37.60%	3.995%

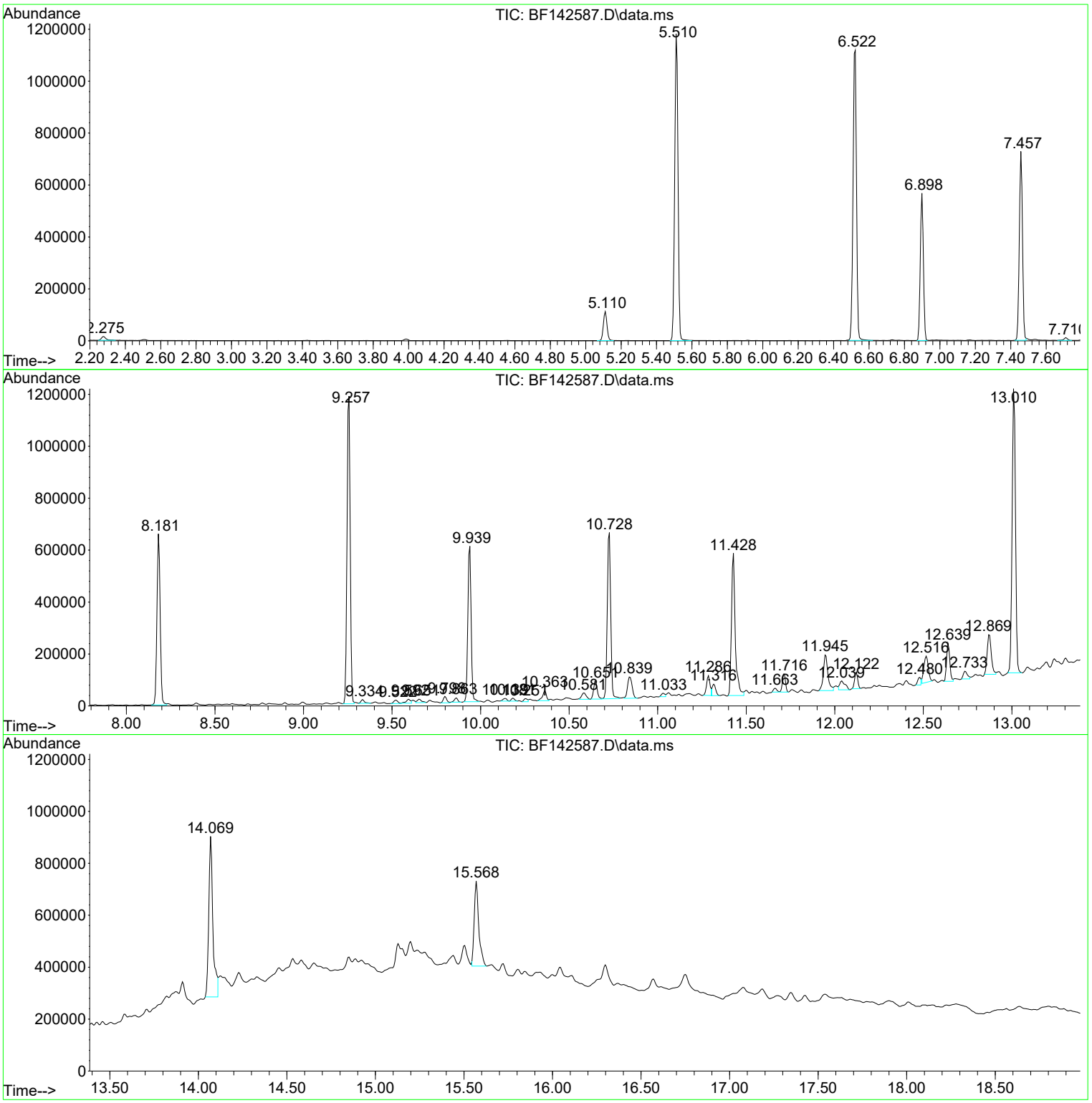
Sum of corrected areas: 14533843

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF053025\
Data File : BF142587.D
Acq On : 30 May 2025 23:41
Operator : RC/JU
Sample : Q2153-01
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TR-04-0592025

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052025.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\BF053025\
Data File : BF142587.D
Acq On : 30 May 2025 23:41
Operator : RC/JU
Sample : Q2153-01
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TR-04-0592025

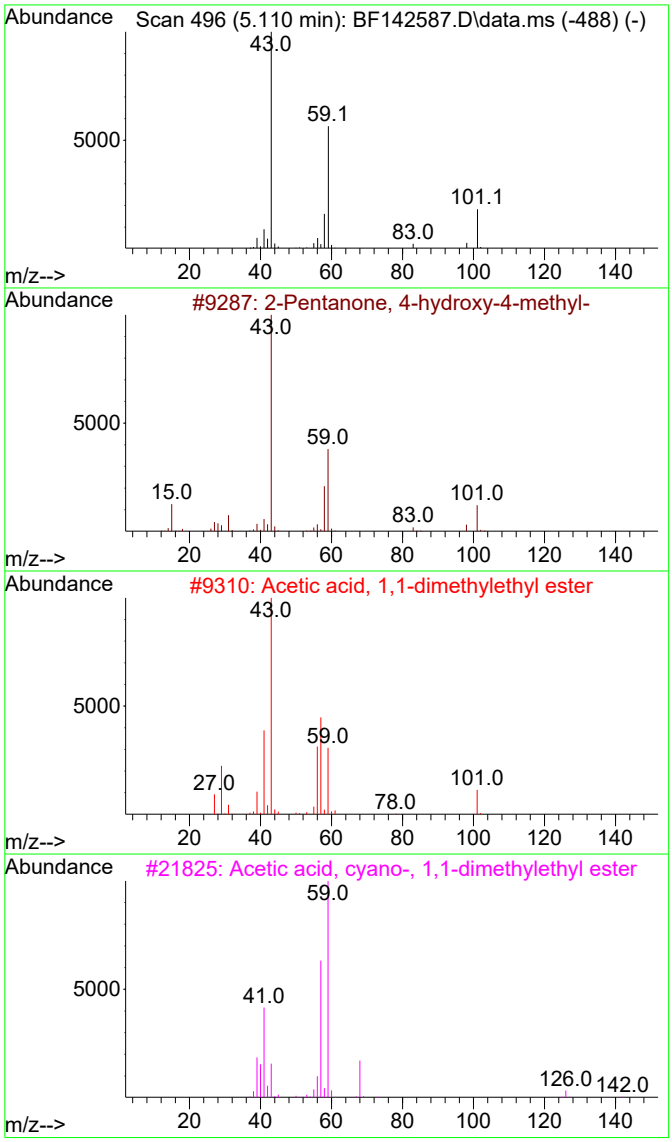
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052025.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

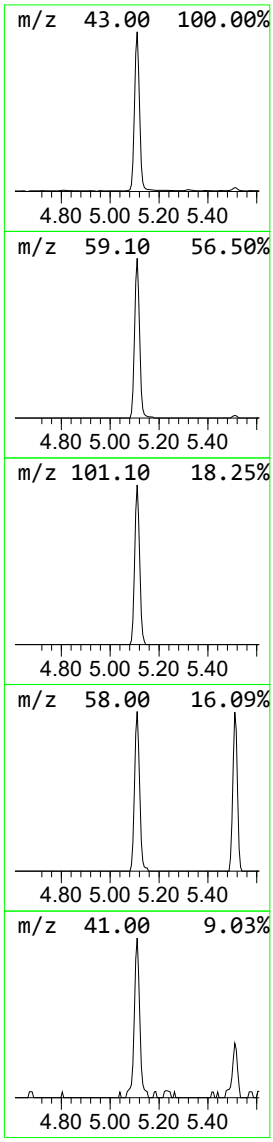
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.110	4.68 ng	160690	1,4-Dichlorobenzene-d4	6.898

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	28
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF053025\
Data File : BF142587.D
Acq On : 30 May 2025 23:41
Operator : RC/JU
Sample : Q2153-01
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TR-04-0592025

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052025.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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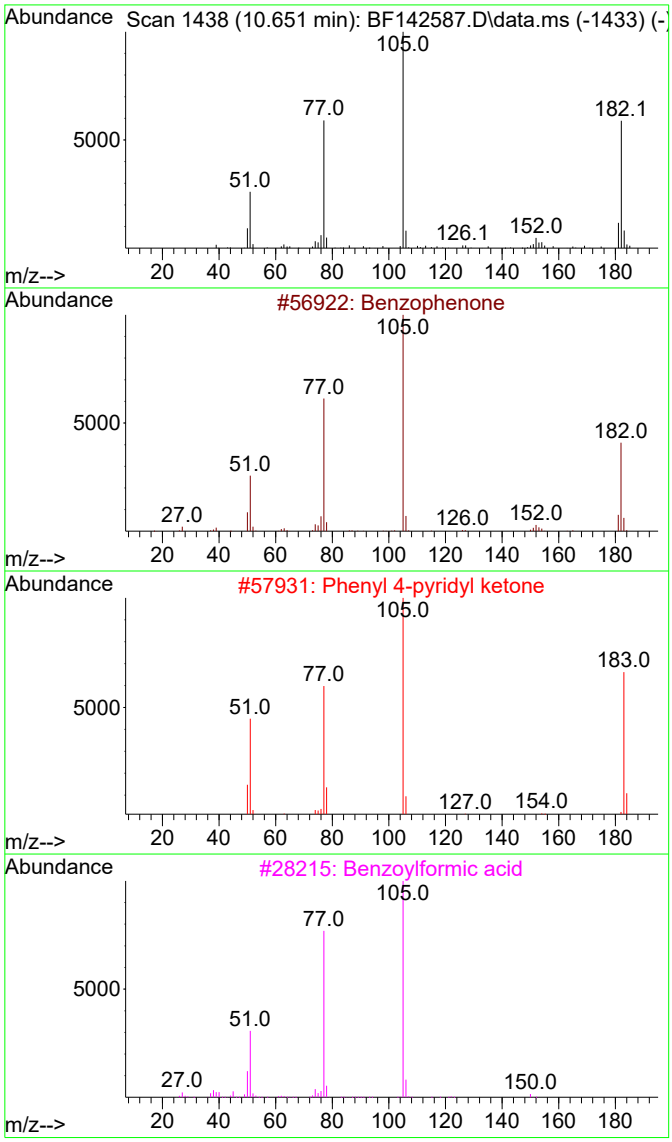
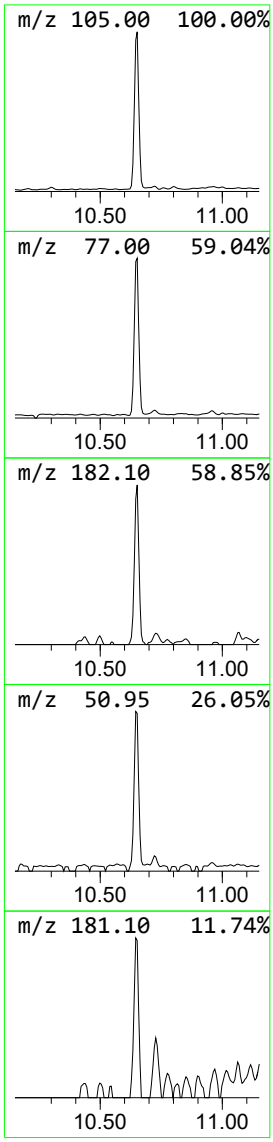
Peak Number 2 Benzophenone Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.651	2.61 ng	101015	Acenaphthene-d10	9.939

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	Phenyl 4-pyridyl ketone	183	C12H9NO	014548-46-0	53
3	Benzoylformic acid	150	C8H6O3	000611-73-4	49
4	Benzenebutanoic acid, .gamma.-oxo-	178	C10H10O3	002051-95-8	47
5	1-Propanone, 3-chloro-1-phenyl-	168	C9H9ClO	000936-59-4	47





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF053025\
Data File : BF142587.D
Acq On : 30 May 2025 23:41
Operator : RC/JU
Sample : Q2153-01
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TR-04-0592025

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052025.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

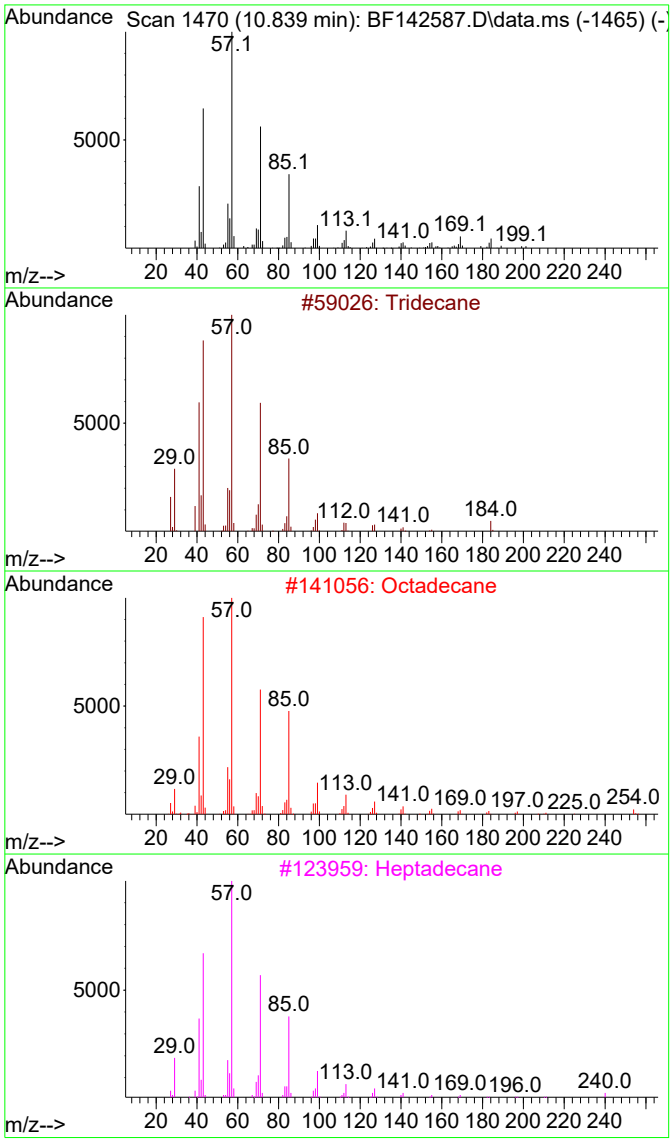
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

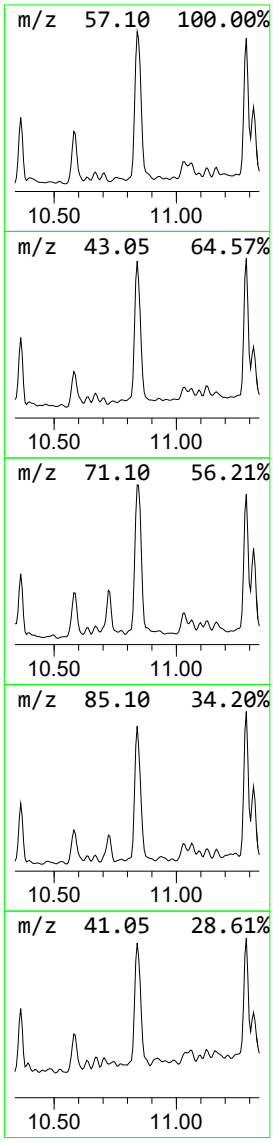
****

Peak Number 3 Tridecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.839	3.67 ng	148661	Phenanthrene-d10	11.428

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane	184	C13H28	000629-50-5	93
2	Octadecane	254	C18H38	000593-45-3	87
3	Heptadecane	240	C17H36	000629-78-7	87
4	Dodecane, 1-iodo-	296	C12H25I	004292-19-7	86
5	Pentadecane	212	C15H32	000629-62-9	83





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF053025\
Data File : BF142587.D
Acq On : 30 May 2025 23:41
Operator : RC/JU
Sample : Q2153-01
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TR-04-0592025

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052025.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

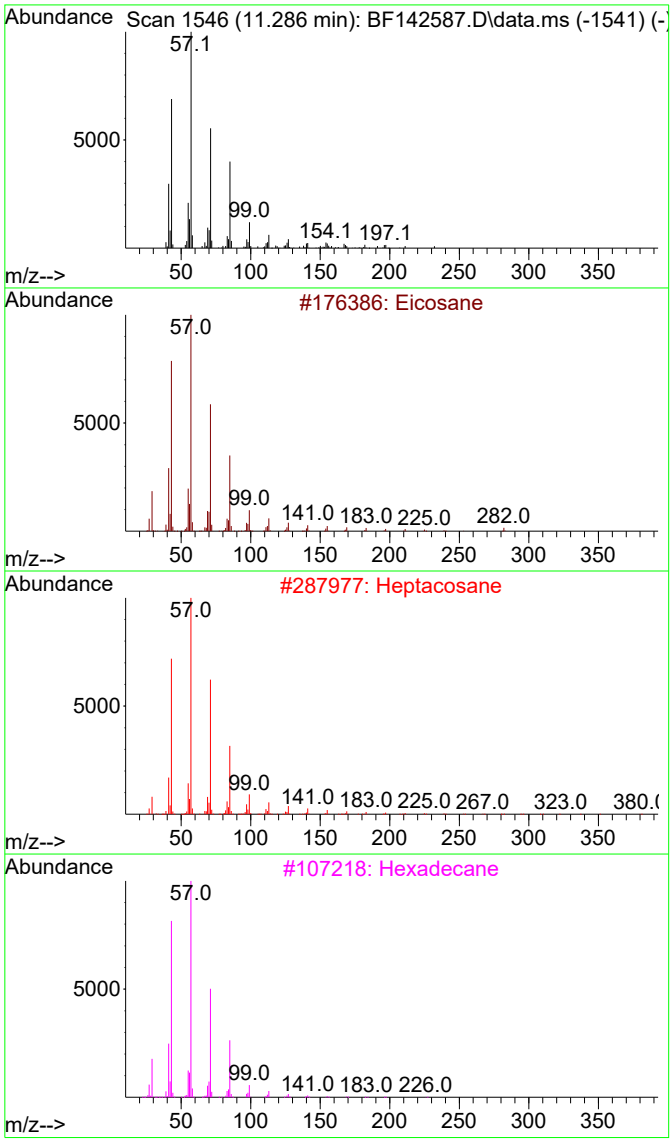
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

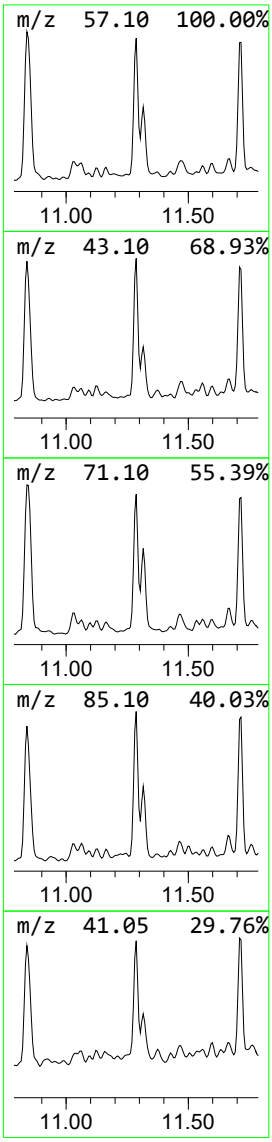
****

Peak Number 4 Eicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.286	2.65 ng	107117	Phenanthrene-d10	11.428

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	91
2	Heptacosane	380	C27H56	000593-49-7	91
3	Hexadecane	226	C16H34	000544-76-3	90
4	Heneicosane	296	C21H44	000629-94-7	90
5	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	90





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF053025\
Data File : BF142587.D
Acq On : 30 May 2025 23:41
Operator : RC/JU
Sample : Q2153-01
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TR-04-0592025

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052025.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

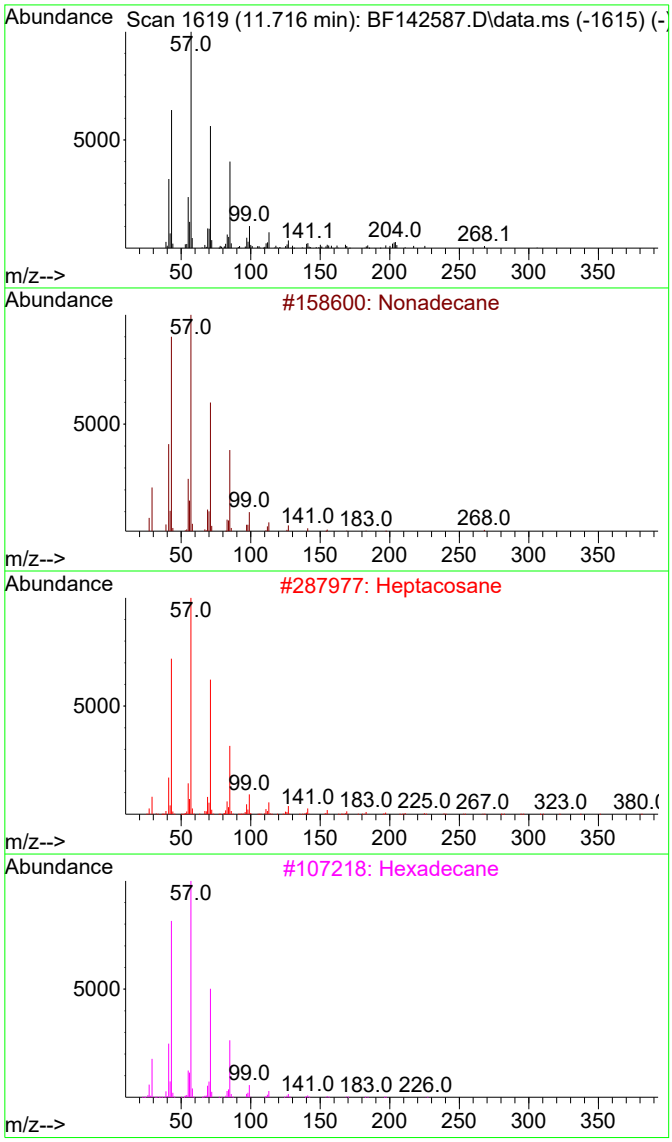
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

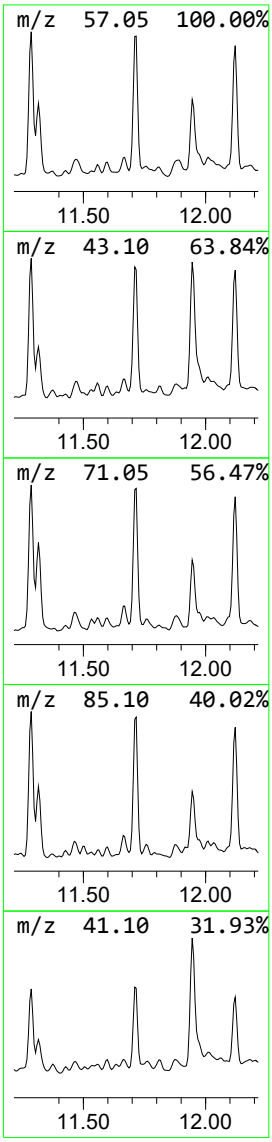
****

Peak Number 5 Nonadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.716	2.13 ng	86143	Phenanthrene-d10	11.428

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane	268	C19H40	000629-92-5	91
2	Heptacosane	380	C27H56	000593-49-7	91
3	Hexadecane	226	C16H34	000544-76-3	90
4	Heneicosane	296	C21H44	000629-94-7	90
5	Eicosane	282	C20H42	000112-95-8	90





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF053025\
Data File : BF142587.D
Acq On : 30 May 2025 23:41
Operator : RC/JU
Sample : Q2153-01
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TR-04-0592025

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052025.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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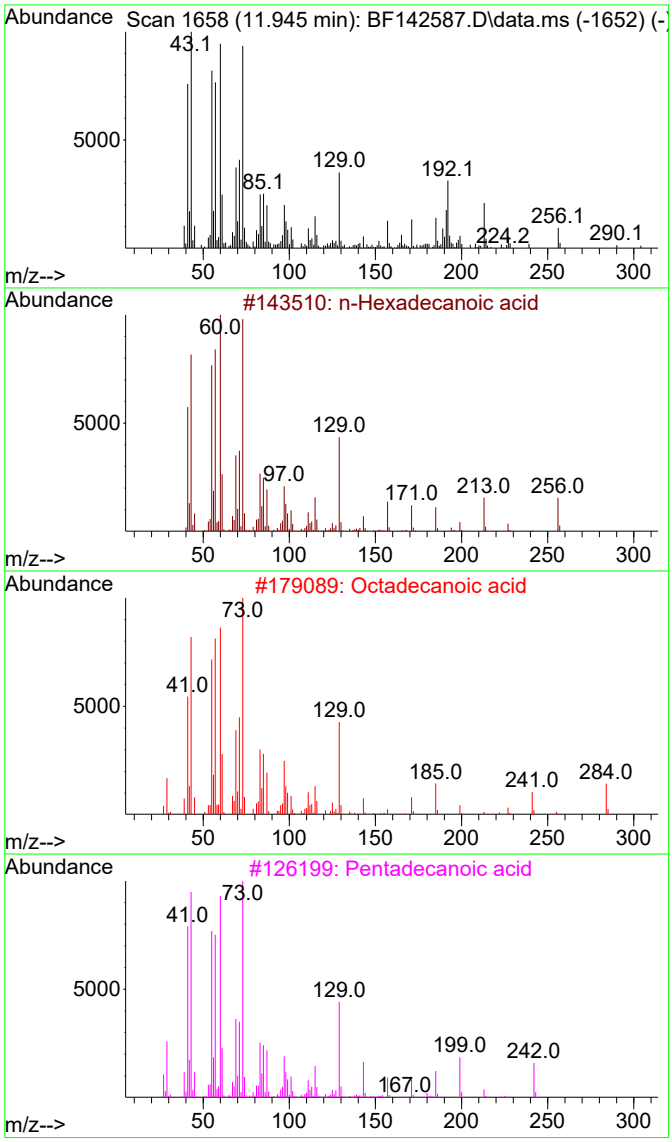
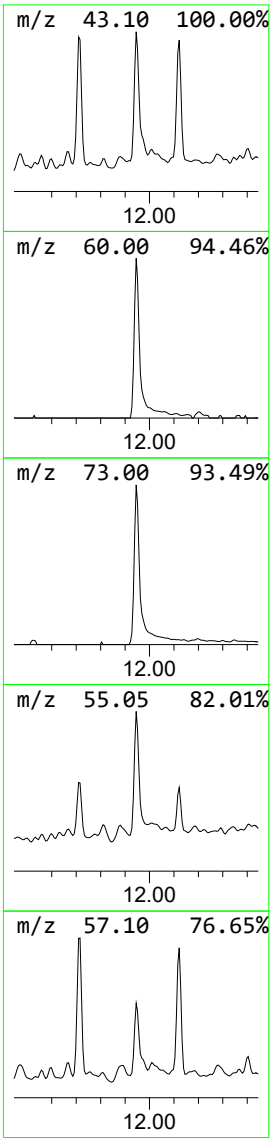
Peak Number 6 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.945	6.12 ng	247619	Phenanthrene-d10	11.428

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Octadecanoic acid	284	C18H36O2	000057-11-4	93
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	83
5	8-Methylnonanoic acid	172	C10H20O2	005963-14-4	70





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF053025\
Data File : BF142587.D
Acq On : 30 May 2025 23:41
Operator : RC/JU
Sample : Q2153-01
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TR-04-0592025

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052025.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

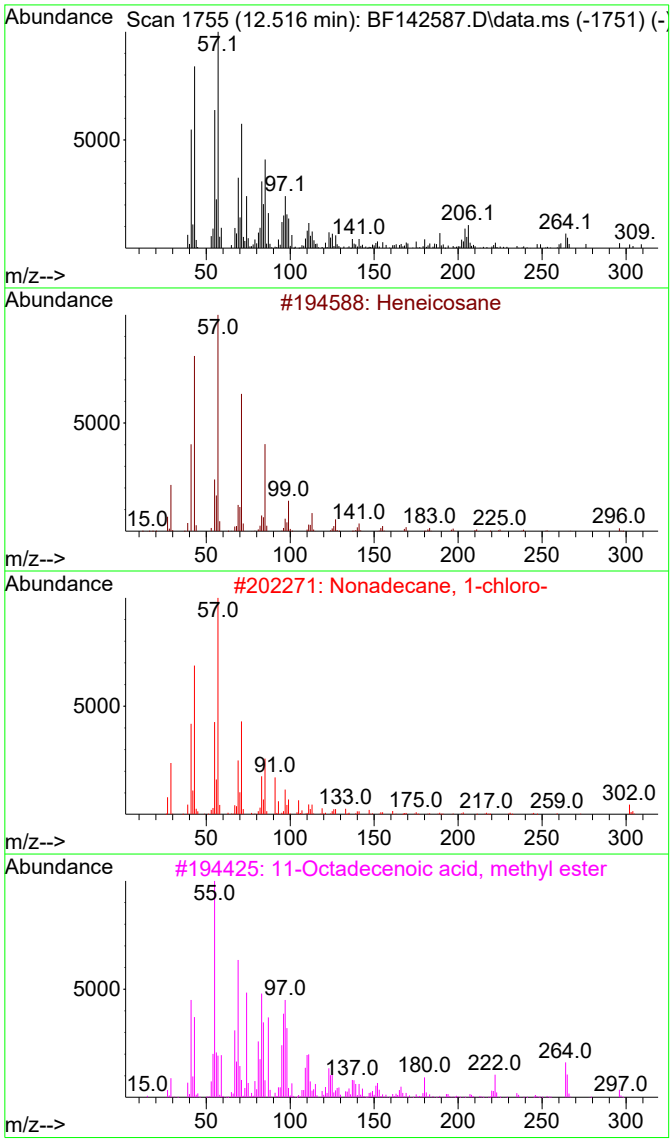
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

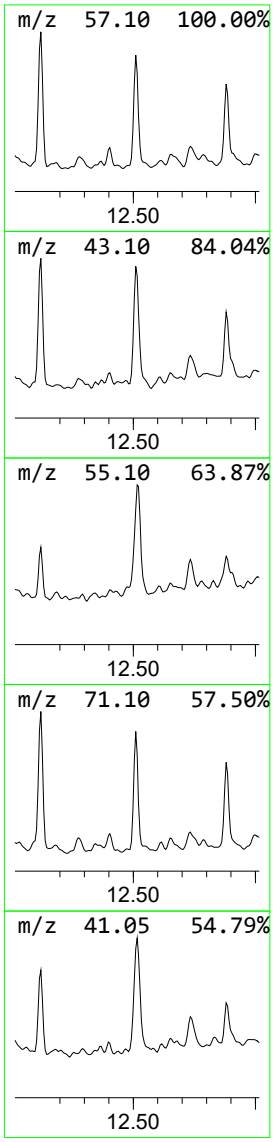
****

Peak Number 7 Heneicosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.516	4.30 ng	174065	Phenanthrene-d10	11.428

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	95
2	Nonadecane, 1-chloro-	302	C19H39Cl	062016-76-6	90
3	11-Octadecenoic acid, methyl ester	296	C19H36O2	052380-33-3	64
4	Hexadecane, 1-chloro-	260	C16H33Cl	004860-03-1	64
5	Sulfurous acid, butyl octadecyl ...	390	C22H46O3S	1000309-18-5	62





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF053025\
Data File : BF142587.D
Acq On : 30 May 2025 23:41
Operator : RC/JU
Sample : Q2153-01
Misc :
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Instrument :
BNA_F
ClientSampleId :
TR-04-0592025

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052025.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
2-Pentanone, 4-...	5.110	4.7	ng	160690	1	6.898	686769	20.0
Benzophenone	10.651	2.6	ng	101015	3	9.939	774318	20.0
Tridecane	10.839	3.7	ng	148661	4	11.428	809606	20.0
Eicosane	11.286	2.6	ng	107117	4	11.428	809606	20.0
Nonadecane	11.716	2.1	ng	86143	4	11.428	809606	20.0
n-Hexadecanoic ...	11.945	6.1	ng	247619	4	11.428	809606	20.0
Heneicosane	12.516	4.3	ng	174065	4	11.428	809606	20.0