LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052125\
Data File : BF142500.D
Acq On : 21 May 2025 21:30
Operator : RC/JU
Sample : Q2052-01
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-B

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: BF142500.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.393	199	204	229	rBV	48753	136964	9.91%	1.158%
2	5.104	488	495	507	rVB	97054	144710	10.47%	1.223%
3	5.510	558	564	580	rVB	809262	1042990	75.48%	8.815%
4	5.781	605	610	619	rBV2	31042	62567	4.53%	0.529%
5	6.134	661	670	678	rBV	46273	71594	5.18%	0.605%
6	6.392	708	714	718	rBV	12588	21226	1.54%	0.179%
7	6.516	729	735	749	rVB	773644	994882	71.99%	8.408%
8	6.722	766	770	776	rBV2	25004	36947	2.67%	0.312%
9	6.898	795	800	806	rVB	403412	491143	35.54%	4.151%
10	7.039	814	824	825	rBV3	8655	17677	1.28%	0.149%
11	7.292	861	867	871	rBV4	9338	17914	1.30%	0.151%
12	7.457	885	895	899	rBV	518777	646008	46.75%	5.460%
13	7.492	899	901	905	rVB	16029	17514	1.27%	0.148%
14	7.710	930	938	944	rVB5	16261	31452	2.28%	0.266%
15	8.181	1010	1018	1025	rBV	410748	519473	37.59%	4.390%
16	8.492	1062	1071	1080	rBV	42983	73758	5.34%	0.623%
17	8.769	1114	1118	1122	rBV	14485	17211	1.25%	0.145%
18	9.257	1196	1201	1206	rBV	834002	1034066	74.83%	8.739%
19	9.333	1210	1214	1222	rVV	25873	37473	2.71%	0.317%
20	9.651	1264	1268	1272	rBV4	12896	19731	1.43%	0.167%
21	9.863	1299	1304	1309	rVB2	22260	31382	2.27%	0.265%
22	9.939	1311	1317	1322	rVV	385364	504344	36.50%	4.262%
23	10.028	1326	1332	1340	rVB	221136	341615	24.72%	2.887%
24	10.363	1383	1389	1393	rBV	25318	38018	2.75%	0.321%
25	10.580	1423	1426	1432	rVB2	10094	14936	1.08%	0.126%
26	10.645	1433	1437	1445	rBV	31425	43838	3.17%	0.370%
27	10.722	1445	1450	1457	rBV	420201	533636	38.62%	4.510%
28	10.845	1466	1471	1479	rVB	29622	51676	3.74%	0.437%
29	11.286	1542	1546	1549	rBV	25384	34245	2.48%	0.289%
30	11.316	1549	1551	1556	rVB2	17112	23060	1.67%	0.195%
31	11.427	1564	1570	1577	rBV	452772	644241	46.62%	5.445%
32	11.716	1615	1619	1622	rBV	18728	22878	1.66%	0.193%
33	11.751	1622	1625	1631	rVB5	11208	16836	1.22%	0.142%
34	11.880	1642	1647	1650	rBV	166824	294059	21.28%	2.485%
35	11.951	1655	1659	1670	rVB2	238019	371801	26.91%	3.142%
36	12.121	1685	1688	1691	rBV	19927	24338	1.76%	0.206%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052125\
Data File : BF142500.D
Acq On : 21 May 2025 21:30
Operator : RC/JU
Sample : Q2052-01
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-B

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	12.163	1691	1695	1701	rVB5	24543	44680	3.23%	0.378%
38	12.457	1742	1745	1751	rBV3	24548	46125	3.34%	0.390%
39	12.516	1752	1755	1760	rVB2	22318	33073	2.39%	0.280%
40	12.639	1772	1776	1779	rBV	117455	156817	11.35%	1.325%
41	12.733	1788	1792	1800	rVB	127535	165458	11.97%	1.398%
42	12.839	1806	1810	1812	rBV3	63610	93297	6.75%	0.788%
43	12.869	1812	1815	1821	rVB	115673	169124	12.24%	1.429%
44	13.010	1834	1839	1847	rVB	1080987	1381898	100.00%	11.679%
45	14.068	2013	2019	2030	rVB2	443874	711097	51.46%	6.010%
46	14.833	2146	2149	2155	rBV3	89925	144226	10.44%	1.219%
47	15.562	2269	2273	2284	rVB	253969	460620	33.33%	3.893%

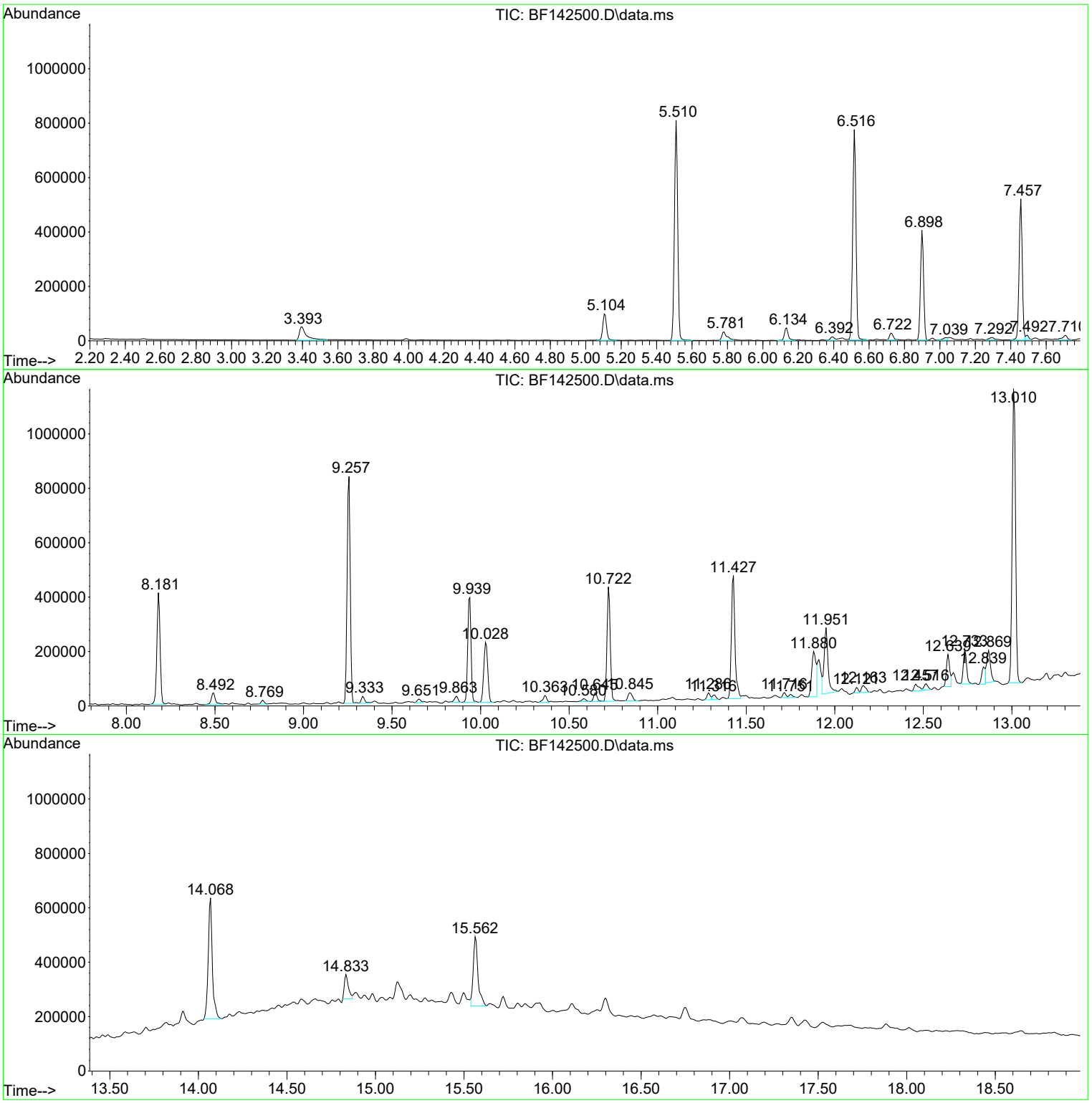
Sum of corrected areas: 11832618

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052125\
Data File : BF142500.D
Acq On : 21 May 2025 21:30
Operator : RC/JU
Sample : Q2052-01
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-B

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\BF052125\
Data File : BF142500.D
Acq On : 21 May 2025 21:30
Operator : RC/JU
Sample : Q2052-01
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-B

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

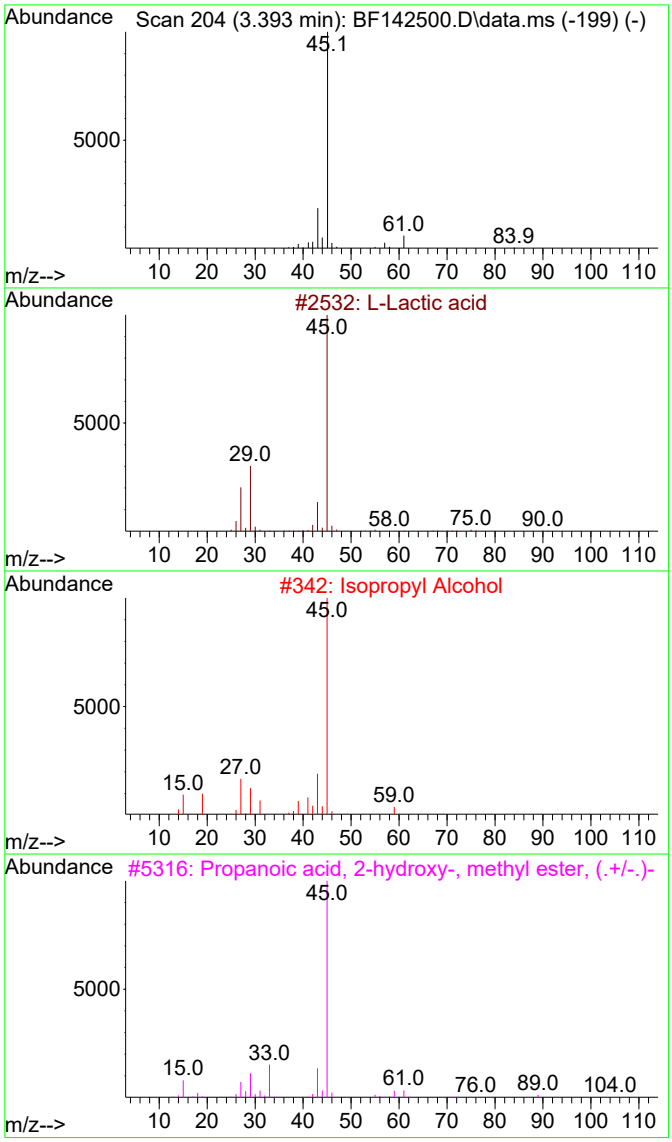
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

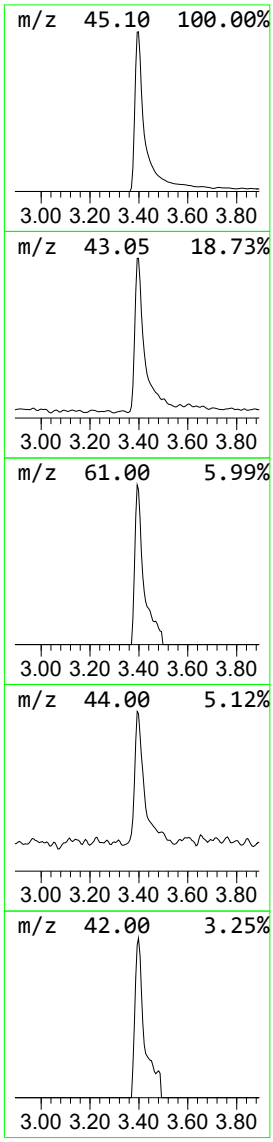
****

Peak Number 1 unknown3.393 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.393	5.58 ng	136964	1,4-Dichlorobenzene-d4	6.898

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	L-Lactic acid	90	C3H6O3	000079-33-4	9
2	Isopropyl Alcohol	60	C3H8O	000067-63-0	9
3	Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	000547-64-8	9
4	Propylene Glycol	76	C3H8O2	000057-55-6	9
5	2-Butanol, 3-methyl-	88	C5H12O	000598-75-4	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052125\
Data File : BF142500.D
Acq On : 21 May 2025 21:30
Operator : RC/JU
Sample : Q2052-01
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-B

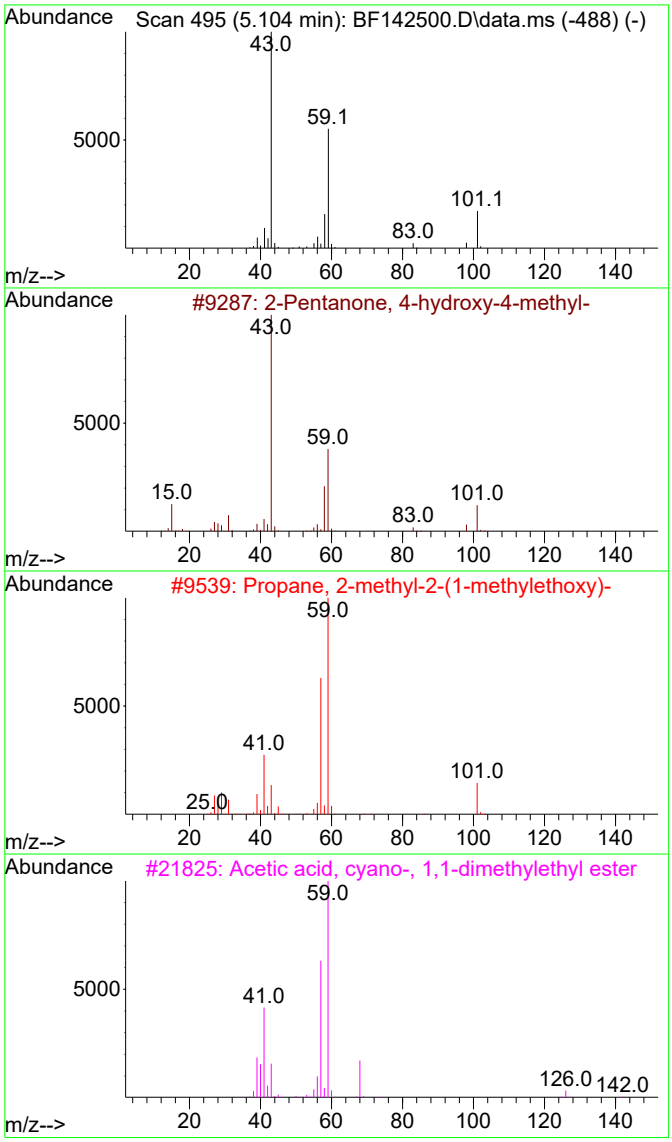
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052025.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

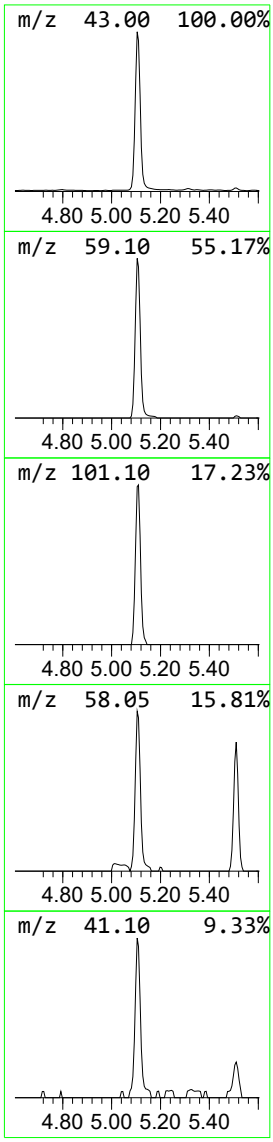
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.104	5.89 ng	144710	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	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052125\
Data File : BF142500.D
Acq On : 21 May 2025 21:30
Operator : RC/JU
Sample : Q2052-01
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-B

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

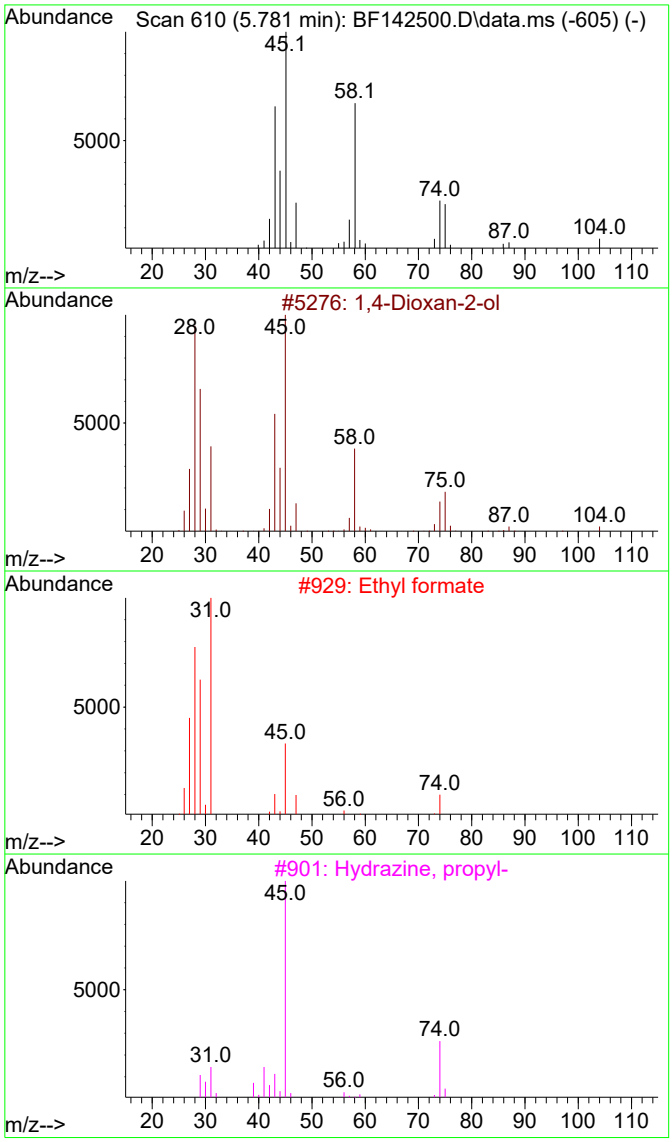
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

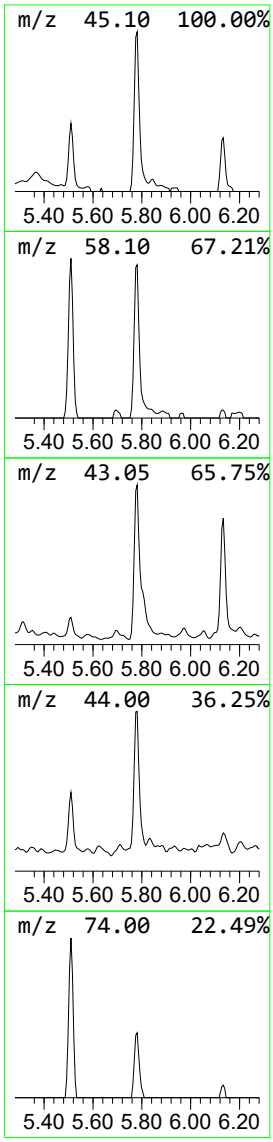
****

Peak Number 3 unknown5.781 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.781	2.55 ng	62567	1,4-Dichlorobenzene-d4	6.898

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,4-Dioxan-2-ol	104	C4H8O3	022347-47-3	49
2	Ethyl formate	74	C3H6O2	000109-94-4	47
3	Hydrazine, propyl-	74	C3H10N2	005039-61-2	43
4	3-Methoxypropionic acid	104	C4H8O3	002544-06-1	38
5	(3-Methyl-oxiran-2-yl)-methanol	88	C4H8O2	1000194-22-9	32





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052125\
Data File : BF142500.D
Acq On : 21 May 2025 21:30
Operator : RC/JU
Sample : Q2052-01
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-B

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

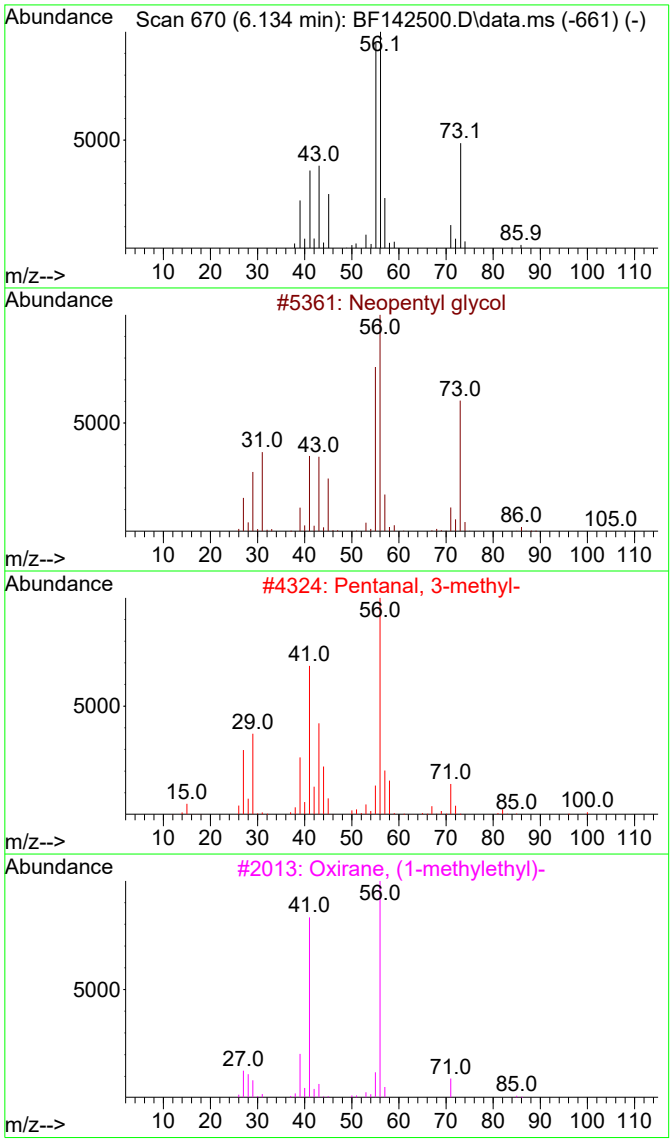
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

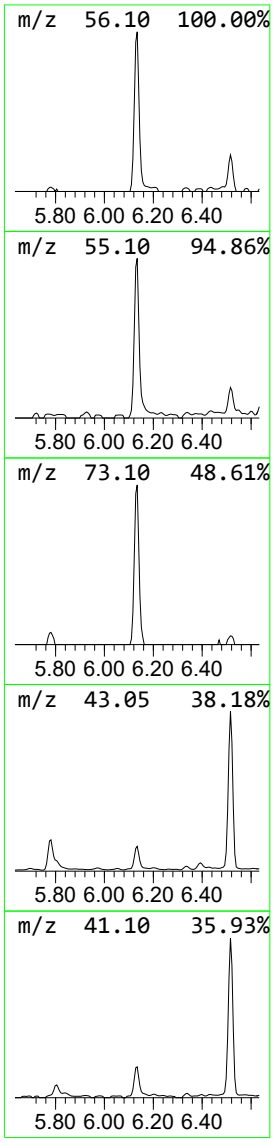
****

Peak Number 4 Neopentyl glycol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.134	2.92 ng	71594	1,4-Dichlorobenzene-d4	6.898

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Neopentyl glycol	104	C5H12O2	000126-30-7	83
2	Pentanal, 3-methyl-	100	C6H12O	015877-57-3	38
3	Oxirane, (1-methylethyl)-	86	C5H10O	001438-14-8	28
4	1-Hepten-4-ol	114	C7H14O	003521-91-3	12
5	Cyclopropylamine	57	C3H7N	000765-30-0	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052125\
Data File : BF142500.D
Acq On : 21 May 2025 21:30
Operator : RC/JU
Sample : Q2052-01
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-B

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

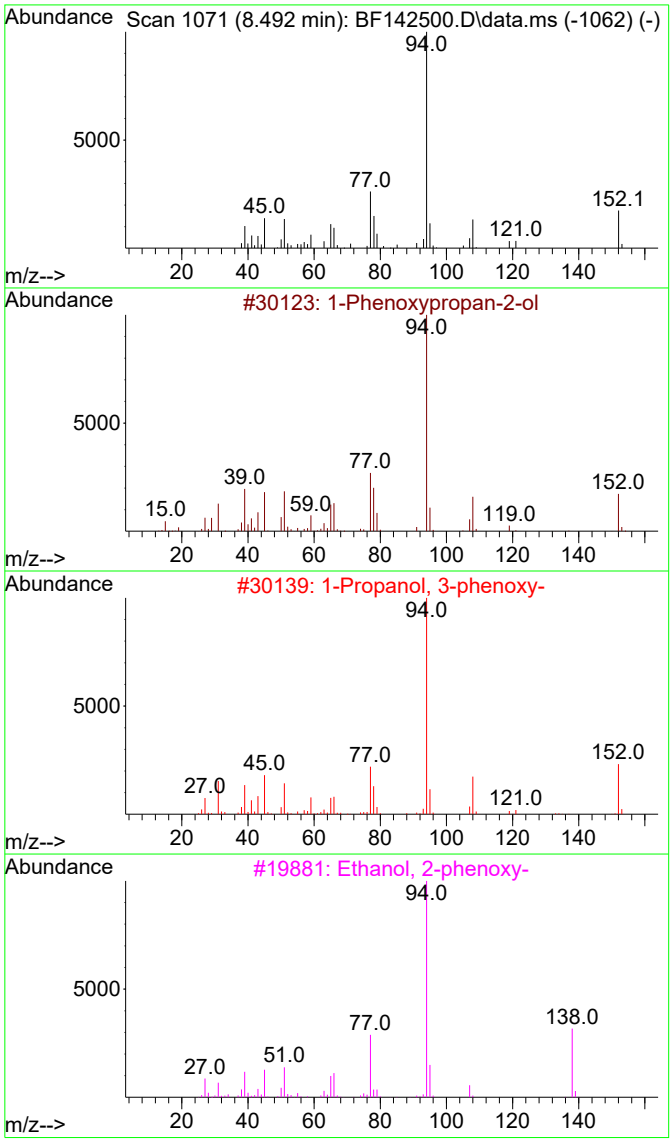
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

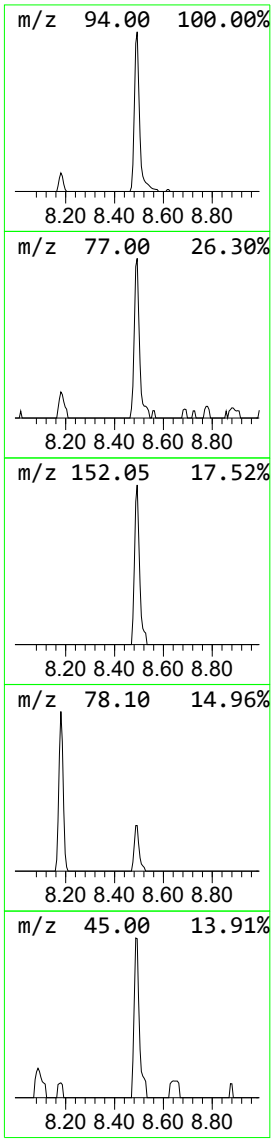
****

Peak Number 5 1-Phenoxypropan-2-ol Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.492	2.84 ng	73758	Naphthalene-d8	8.181

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	96
2	1-Propanol, 3-phenoxy-	152	C9H12O2	006180-61-6	87
3	Ethanol, 2-phenoxy-	138	C8H10O2	000122-99-6	64
4	1-Propanol, 2-phenoxy-	152	C9H12O2	004169-04-4	59
5	2-Hexen-4-yne, 2-methyl-	94	C7H10	058275-93-7	53





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052125\
Data File : BF142500.D
Acq On : 21 May 2025 21:30
Operator : RC/JU
Sample : Q2052-01
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_F
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TP-B

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

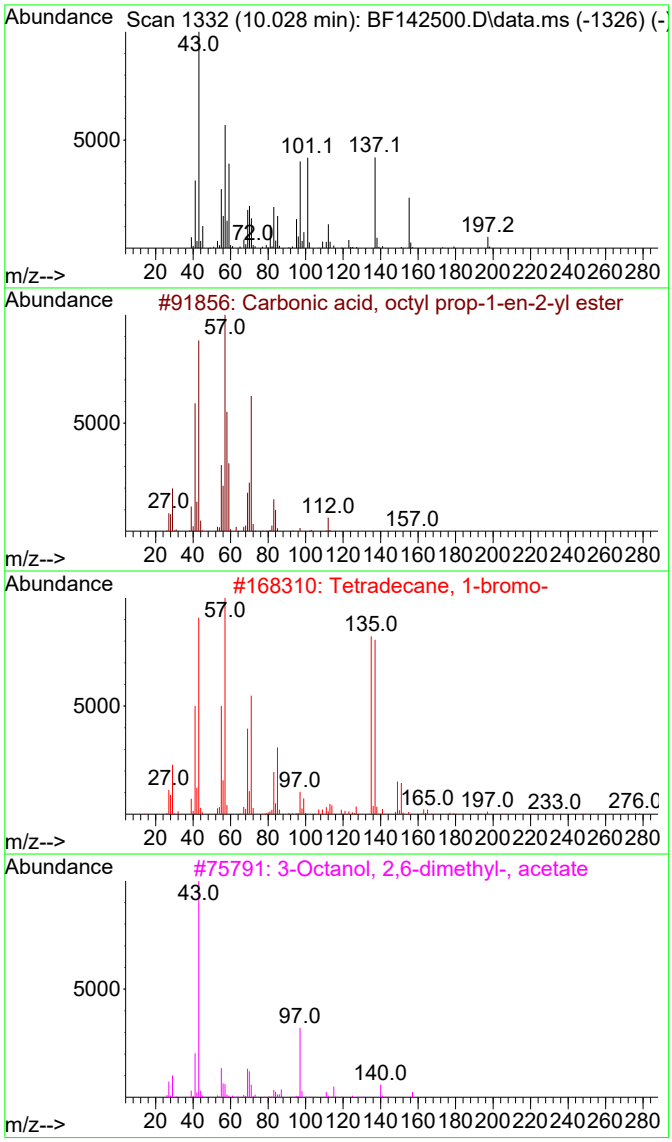
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

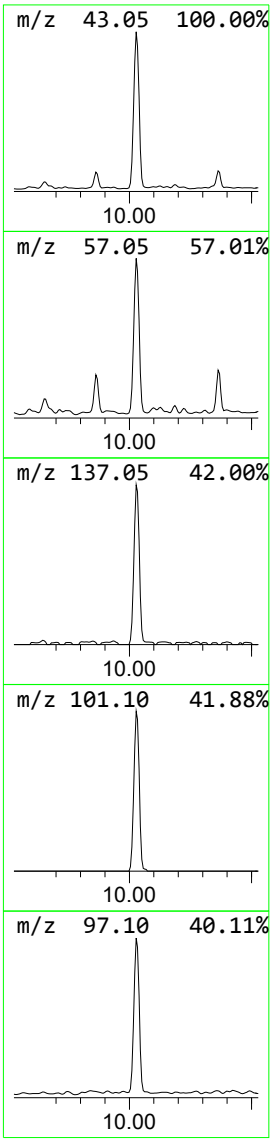
****

Peak Number 6 unknown10.028 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.028	13.55 ng	341615	Acenaphthene-d10	9.939

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Carbonic acid, octyl prop-1-en-2...	214	C12H22O3	1000382-54-0	12
2	Tetradecane, 1-bromo-	276	C14H29Br	000112-71-0	10
3	3-Octanol, 2,6-dimethyl-, acetate	200	C12H24O2	123232-57-5	10
4	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	10
5	Carbonic acid, eicosyl prop-1-en...	382	C24H46O3	1000383-10-8	9





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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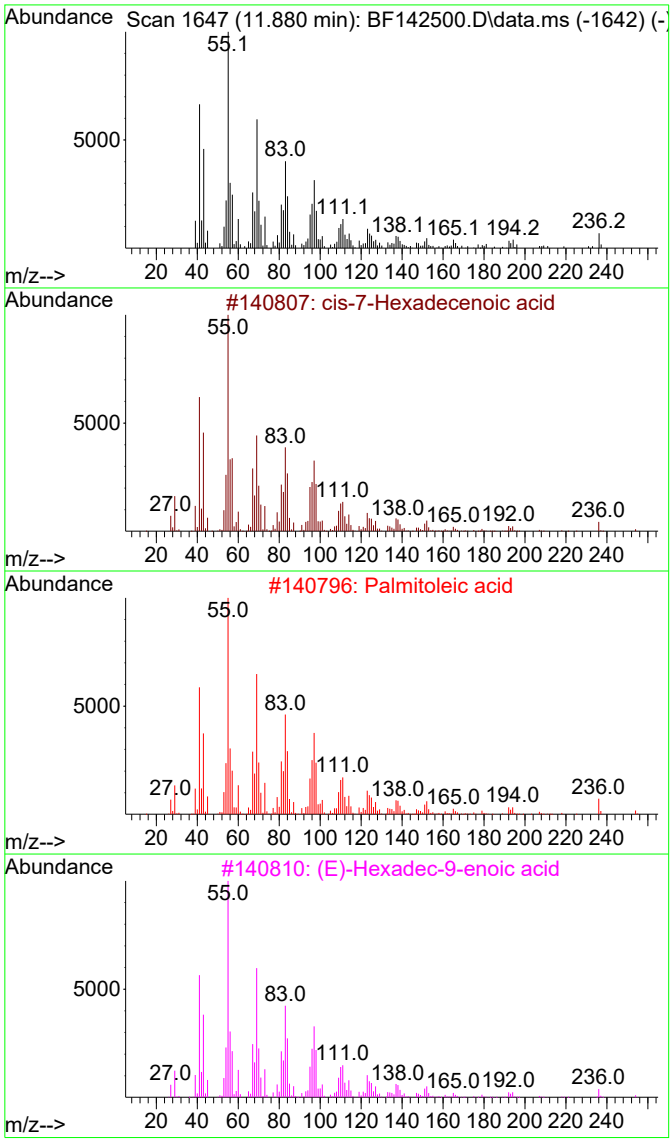
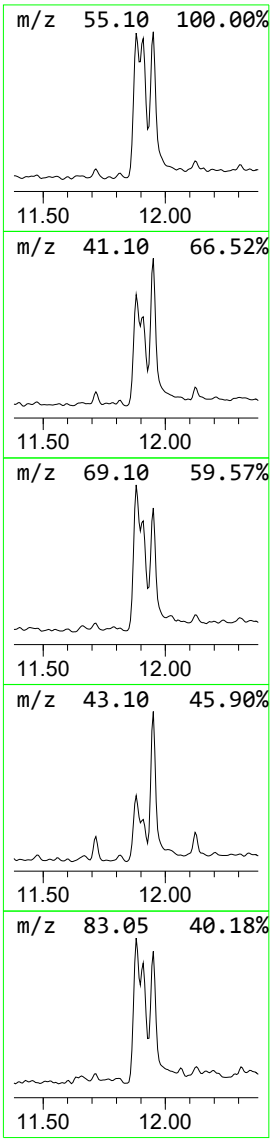
Peak Number 7 cis-7-Hexadecenoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.880	9.13 ng	294059	Phenanthrene-d10	11.427

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	cis-7-Hexadecenoic acid	254	C16H30O2	002416-19-5	94
2	Palmitoleic acid	254	C16H30O2	000373-49-9	93
3	(E)-Hexadec-9-enoic acid	254	C16H30O2	010030-73-6	93
4	Hexadecenoic acid, Z-11-	254	C16H30O2	002416-20-8	91
5	E-9-Tetradecenoic acid	226	C14H26O2	050286-30-1	68





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052125\
Data File : BF142500.D
Acq On : 21 May 2025 21:30
Operator : RC/JU
Sample : Q2052-01
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-B

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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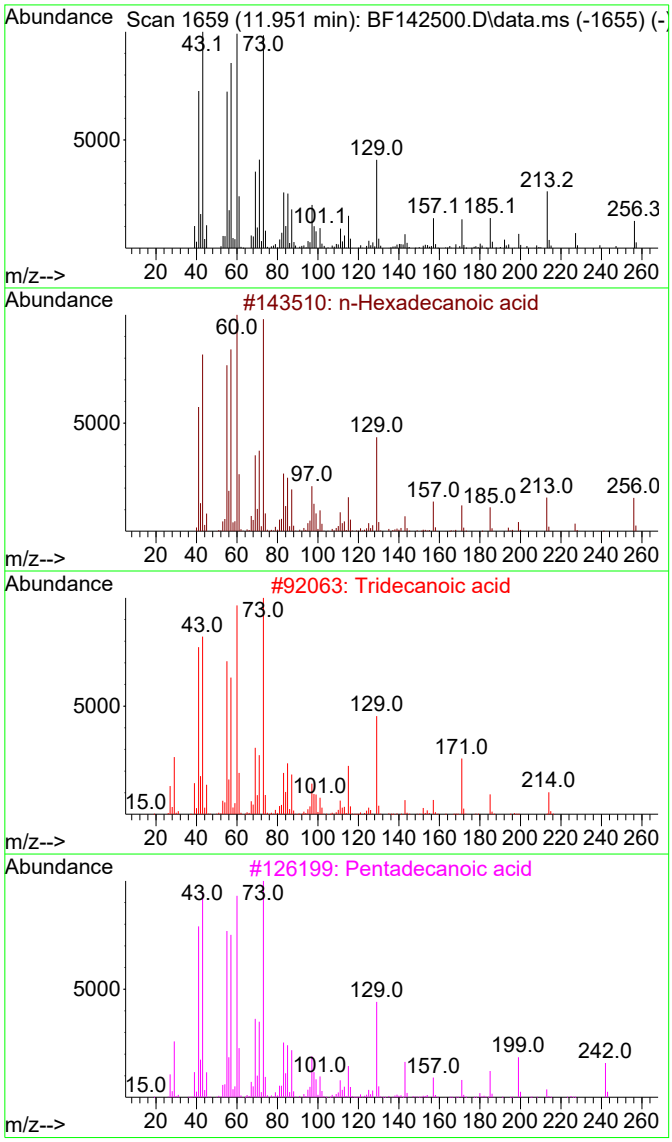
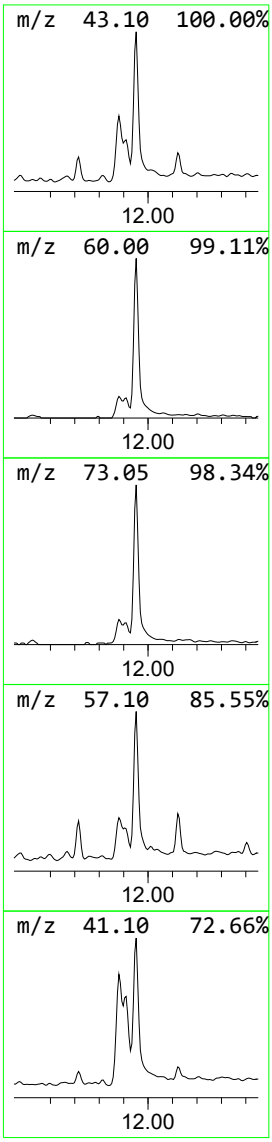
Peak Number 8 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.951	11.54 ng	371801	Phenanthrene-d10	11.427

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	87
5	Dodecanoic acid	200	C12H24O2	000143-07-7	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052125\
Data File : BF142500.D
Acq On : 21 May 2025 21:30
Operator : RC/JU
Sample : Q2052-01
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-B

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

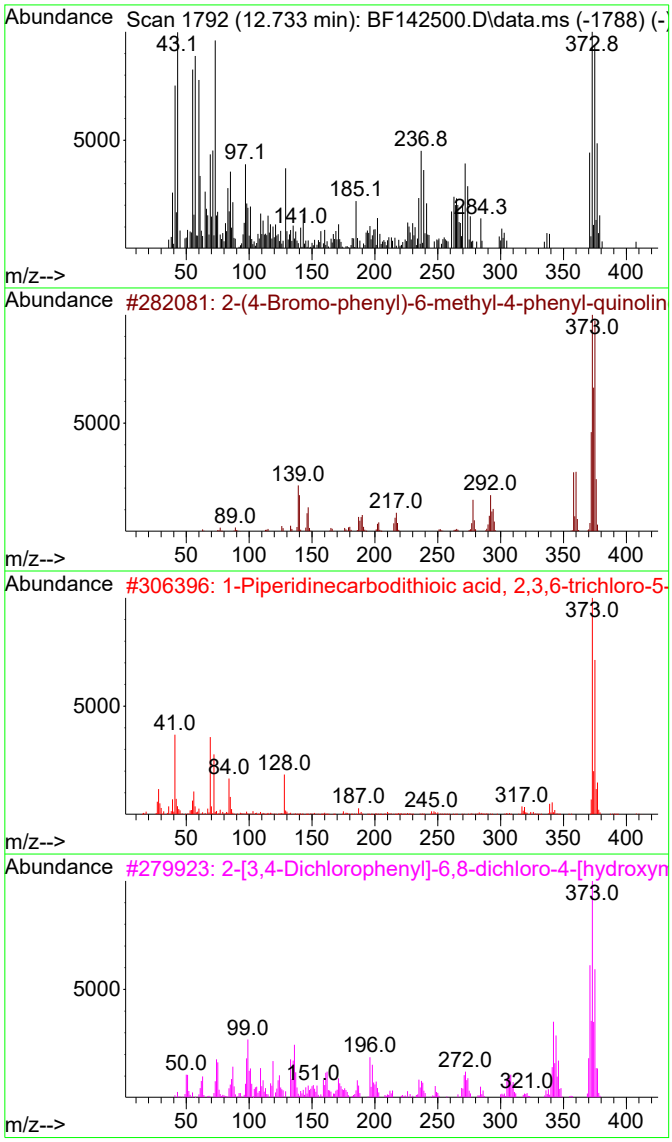
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

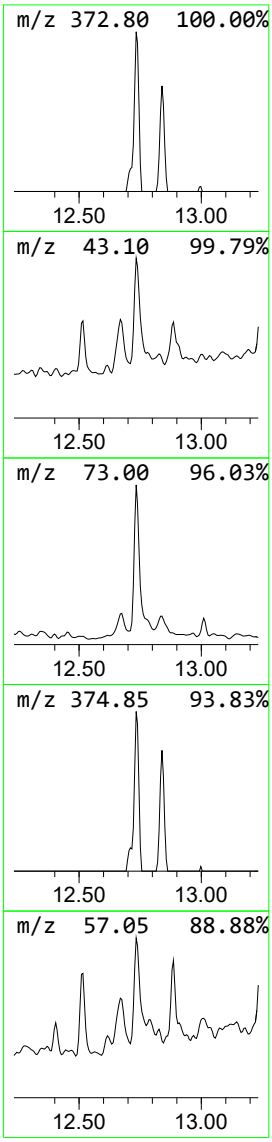
****

Peak Number 9 unknown12.733 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.733	5.14 ng	165458	Phenanthrene-d10	11.427

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-(4-Bromo-phenyl)-6-methyl-4-ph...	373	C22H16BrN	071858-09-8	17
2	1-Piperidinecarbodithioic acid, ...	408	C12H10Cl3F3N2S2	1000305-31-5	16
3	2-[3,4-Dichlorophenyl]-6,8-dichl...	371	C16H9Cl4NO	038599-01-8	12
4	4-Morpholinecarbodithioic acid, ...	410	C11H8Cl3F3N2OS2	1000305-31-7	12
5	tert-Butyldimethylsilyl 4-((tert...	430	C20H35ClO4Si2	1000385-75-1	10





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052125\
Data File : BF142500.D
Acq On : 21 May 2025 21:30
Operator : RC/JU
Sample : Q2052-01
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-B

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

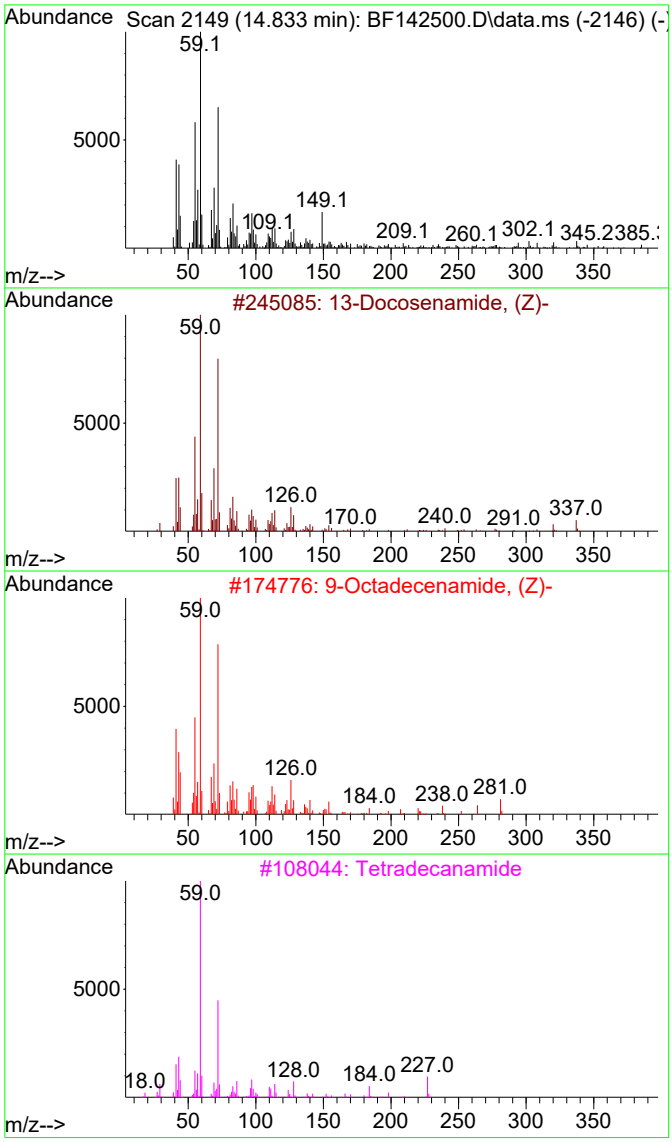
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

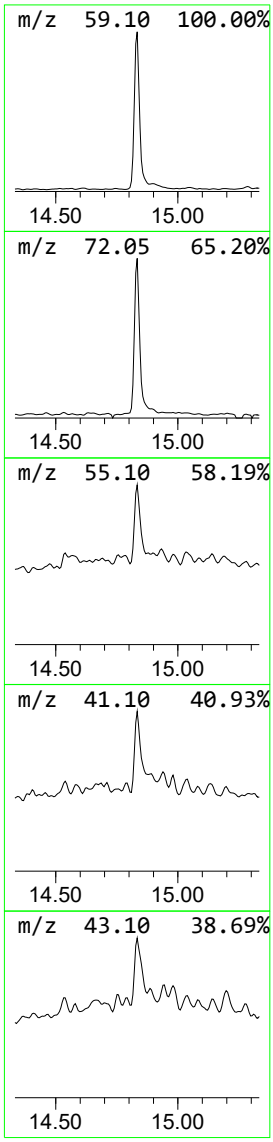
****

Peak Number 10 13-Docosenamide, (Z)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.833	6.26 ng	144226	Perylene-d12	15.563

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	96
2	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	93
3	Tetradecanamide	227	C14H29NO	000638-58-4	72
4	Palmitoleamide	253	C16H31NO	106010-22-4	38
5	1,3-Dioxolo[4,5-c]pyran-7-ol, te...	286	C14H22O6	1000195-94-3	38





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052125\
Data File : BF142500.D
Acq On : 21 May 2025 21:30
Operator : RC/JU
Sample : Q2052-01
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-B

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
unknown3.393	3.393	5.6	ng	136964	1	6.898	491143	20.0
2-Pentanone, 4-...	5.104	5.9	ng	144710	1	6.898	491143	20.0
unknown5.781	5.781	2.5	ng	62567	1	6.898	491143	20.0
Neopentyl glycol	6.134	2.9	ng	71594	1	6.898	491143	20.0
1-Phenoxypropan...	8.492	2.8	ng	73758	2	8.181	519473	20.0
unknown10.028	10.028	13.6	ng	341615	3	9.939	504344	20.0
cis-7-Hexadecen...	11.880	9.1	ng	294059	4	11.427	644241	20.0
n-Hexadecanoic ...	11.951	11.5	ng	371801	4	11.427	644241	20.0
unknown12.733	12.733	5.1	ng	165458	4	11.427	644241	20.0
13-Docosenamide...	14.833	6.3	ng	144226	6	15.563	460620	20.0