LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052225\
Data File : BF142512.D
Acq On : 22 May 2025 16:04
Operator : RC/JU
Sample : Q2052-01
Misc :
ALS Vial : 12 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: BF142512.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.404	199	206	225	rBV	84276	204644	13.80%	1.455%
2	5.104	488	495	503	rVB	123933	183703	12.38%	1.306%
3	5.510	558	564	580	rVB	1034713	1351132	91.09%	9.604%
4	5.775	604	609	618	rBV2	43428	83928	5.66%	0.597%
5	6.134	661	670	678	rBV	67327	104474	7.04%	0.743%
6	6.398	711	715	720	rBV	20628	35849	2.42%	0.255%
7	6.516	729	735	744	rVB	1071056	1398679	94.30%	9.942%
8	6.722	765	770	775	rBV3	35636	48641	3.28%	0.346%
9	6.898	794	800	805	rVB	512399	629870	42.46%	4.477%
10	7.034	816	823	824	rBV3	11815	20561	1.39%	0.146%
11	7.292	860	867	871	rBV4	13590	25163	1.70%	0.179%
12	7.457	884	895	899	rBV	708545	914262	61.64%	6.498%
13	7.487	899	900	905	rVB	19248	19153	1.29%	0.136%
14	7.704	929	937	945	rVB5	23883	48877	3.30%	0.347%
15	8.181	1010	1018	1025	rBV	579602	751177	50.64%	5.339%
16	8.486	1061	1070	1079	rBV	68141	114595	7.73%	0.815%
17	8.769	1113	1118	1122	rBV	21387	27017	1.82%	0.192%
18	9.251	1195	1200	1205	rBV	1191925	1483276	100.00%	10.543%
19	9.333	1209	1214	1218	rVV	35641	47809	3.22%	0.340%
20	9.398	1222	1225	1230	rVB6	11462	17384	1.17%	0.124%
21	9.592	1251	1258	1260	rBV5	9083	19986	1.35%	0.142%
22	9.651	1264	1268	1271	rBV3	15441	22483	1.52%	0.160%
23	9.857	1299	1303	1308	rVB2	32207	45726	3.08%	0.325%
24	9.933	1311	1316	1321	rVV	540990	662754	44.68%	4.711%
25	10.028	1326	1332	1339	rVB	308131	465086	31.36%	3.306%
26	10.363	1382	1389	1392	rBV	33676	48718	3.28%	0.346%
27	10.580	1421	1426	1432	rVB	14684	24694	1.66%	0.176%
28	10.645	1432	1437	1444	rBV	44367	61791	4.17%	0.439%
29	10.722	1445	1450	1455	rBV	468641	592831	39.97%	4.214%
30	10.839	1465	1470	1479	rVB	42393	76816	5.18%	0.546%
31	11.286	1542	1546	1548	rBV	27776	37735	2.54%	0.268%
32	11.316	1548	1551	1556	rVB	19613	27472	1.85%	0.195%
33	11.422	1564	1569	1576	rBV	523755	716064	48.28%	5.090%
34	11.710	1615	1618	1621	rBV	21877	25602	1.73%	0.182%
35	11.745	1621	1624	1630	rVB5	12795	18598	1.25%	0.132%
36	11.874	1641	1646	1649	rBV	144884	251452	16.95%	1.787%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052225\
Data File : BF142512.D
Acq On : 22 May 2025 16:04
Operator : RC/JU
Sample : Q2052-01
Misc :
ALS Vial : 12 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	11.945	1655	1658	1670	rVB2	195744	275617	18.58%	1.959%
38	12.122	1684	1688	1691	rBV	21866	30046	2.03%	0.214%
39	12.157	1691	1694	1701	rVB6	27051	49139	3.31%	0.349%
40	12.451	1741	1744	1750	rBV3	22506	41935	2.83%	0.298%
41	12.510	1751	1754	1759	rVB3	21520	32815	2.21%	0.233%
42	12.633	1771	1775	1778	rBV	114706	152117	10.26%	1.081%
43	12.727	1787	1791	1798	rVB2	102685	131813	8.89%	0.937%
44	12.833	1805	1809	1811	rBV3	67450	97849	6.60%	0.695%
45	12.863	1811	1814	1821	rVB	111588	166704	11.24%	1.185%
46	13.004	1833	1838	1846	rVB	996327	1320971	89.06%	9.389%
47	14.063	2013	2018	2029	rVB2	409341	632918	42.67%	4.499%
48	14.827	2145	2148	2153	rBV3	61064	92007	6.20%	0.654%
49	15.557	2267	2272	2282	rVB	244771	437076	29.47%	3.107%

Sum of corrected areas: 14069009

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052225\
Data File : BF142512.D
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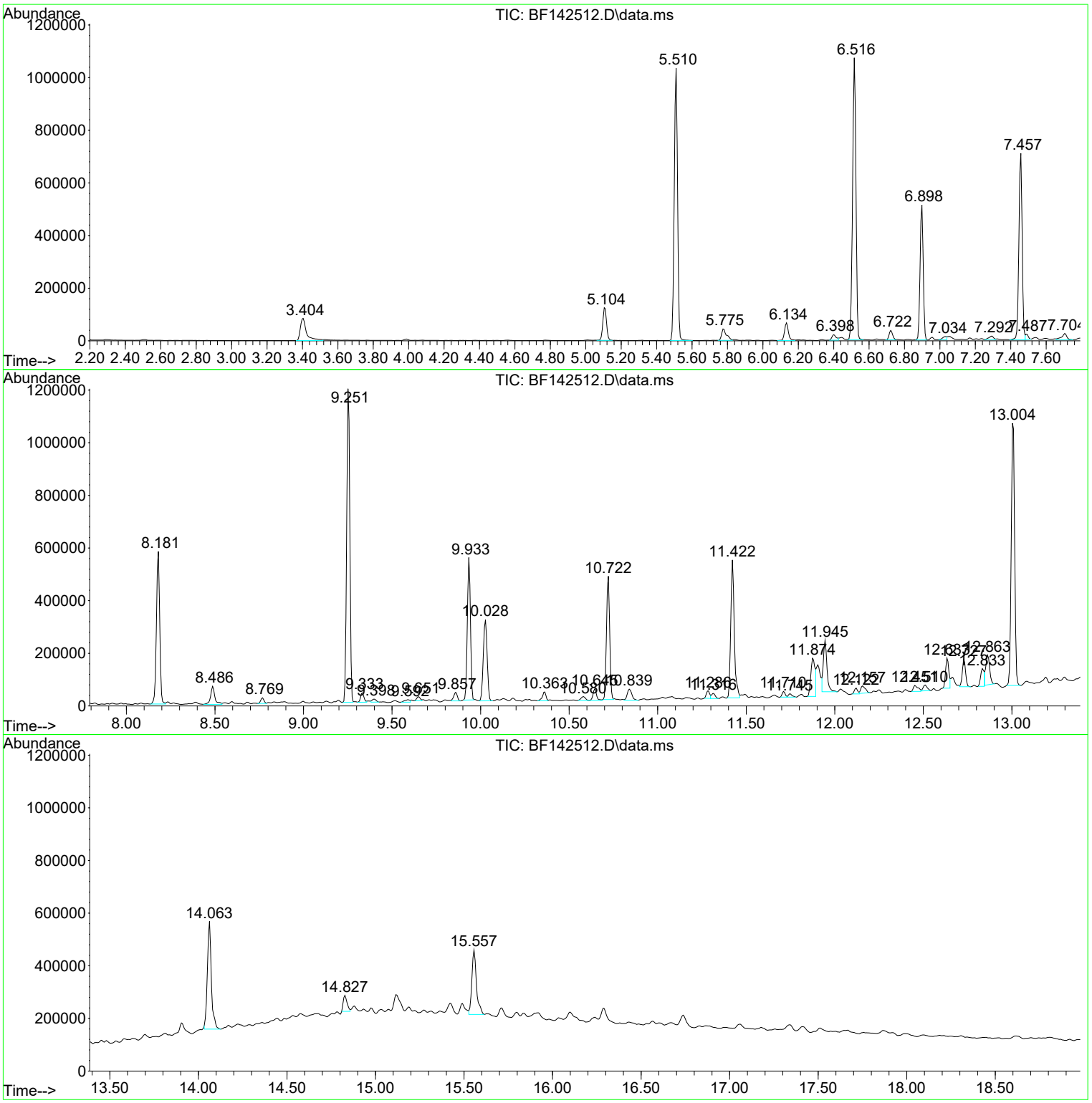
Instrument :
BNA_F
ClientSampleId :
TP-B

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\BF052225\
Data File : BF142512.D
Acq On : 22 May 2025 16:04
Operator : RC/JU
Sample : Q2052-01
Misc :
ALS Vial : 12 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

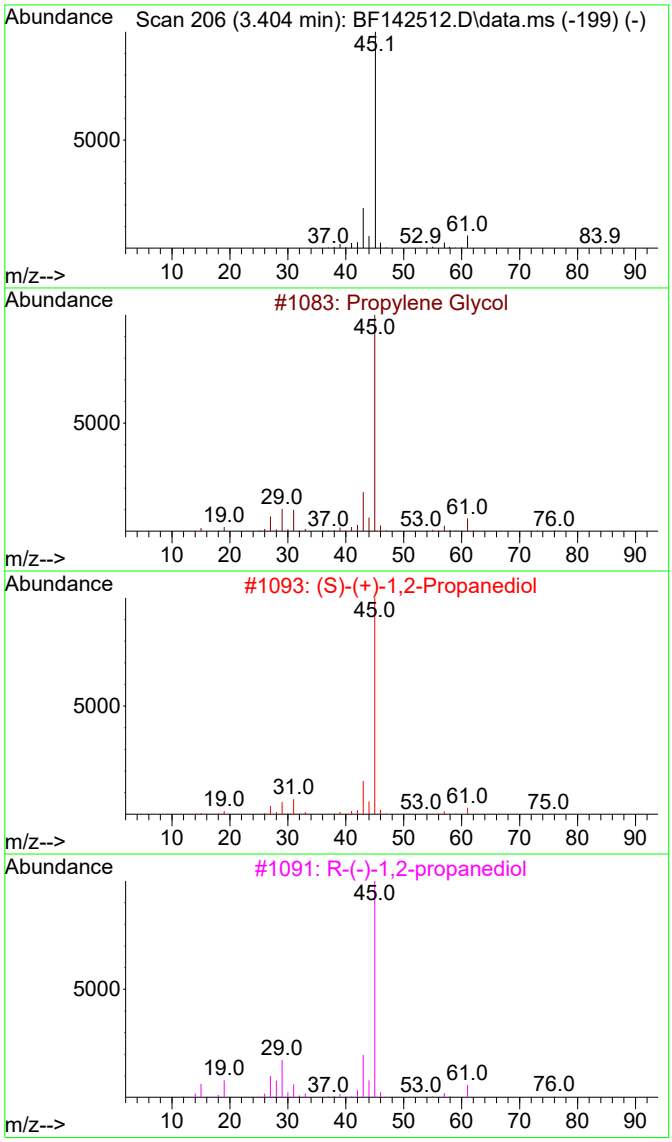
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

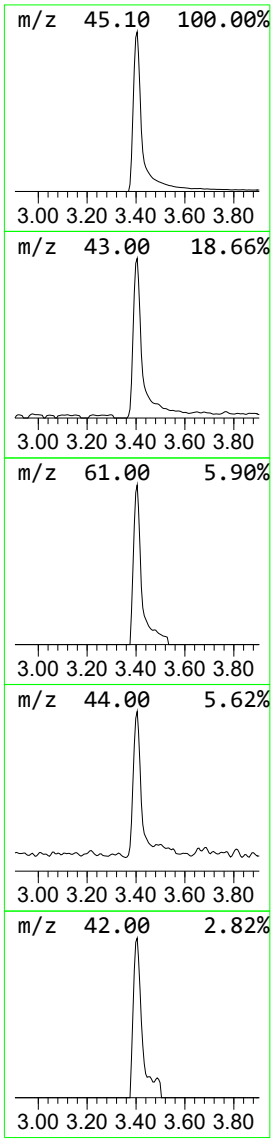
****

Peak Number 1 Propylene Glycol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.404	6.50 ng	204644	1,4-Dichlorobenzene-d4	6.898

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propylene Glycol	76	C3H8O2	000057-55-6	74
2	(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	64
3	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	43
4	Isopropyl Alcohol	60	C3H8O	000067-63-0	9
5	Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	000547-64-8	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052225\
Data File : BF142512.D
Acq On : 22 May 2025 16:04
Operator : RC/JU
Sample : Q2052-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-B

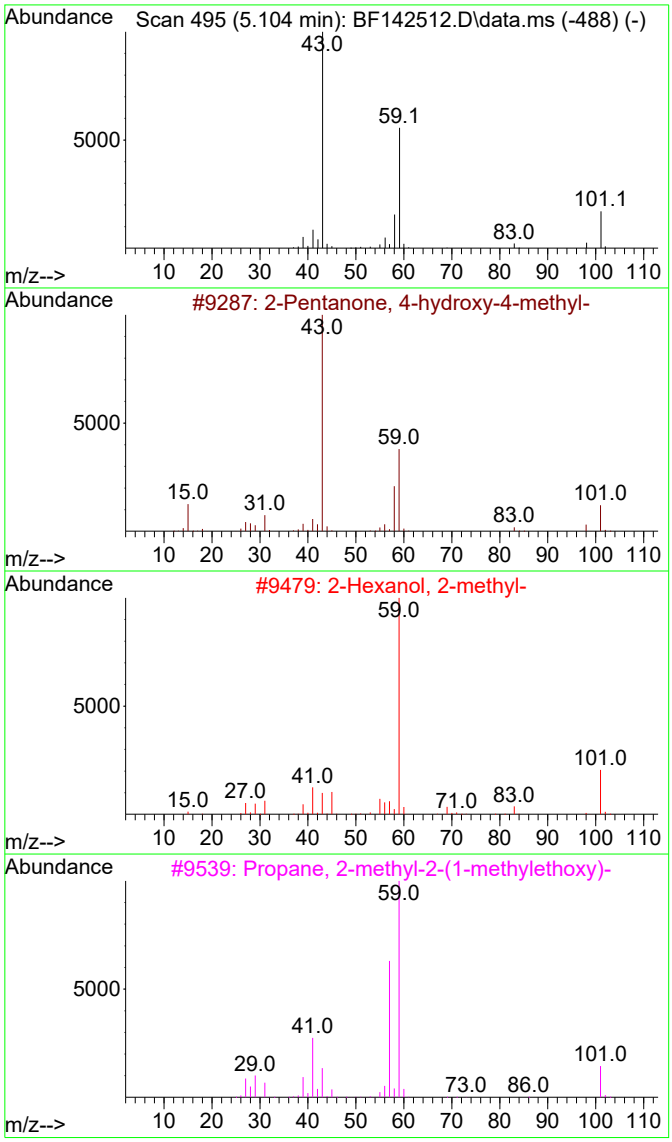
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052025.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

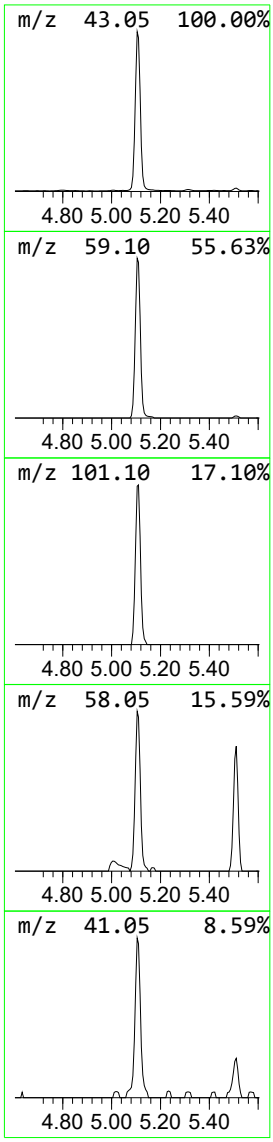
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.104	5.83 ng	183703	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	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
3	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	33
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052225\
Data File : BF142512.D
Acq On : 22 May 2025 16:04
Operator : RC/JU
Sample : Q2052-01
Misc :
ALS Vial : 12 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

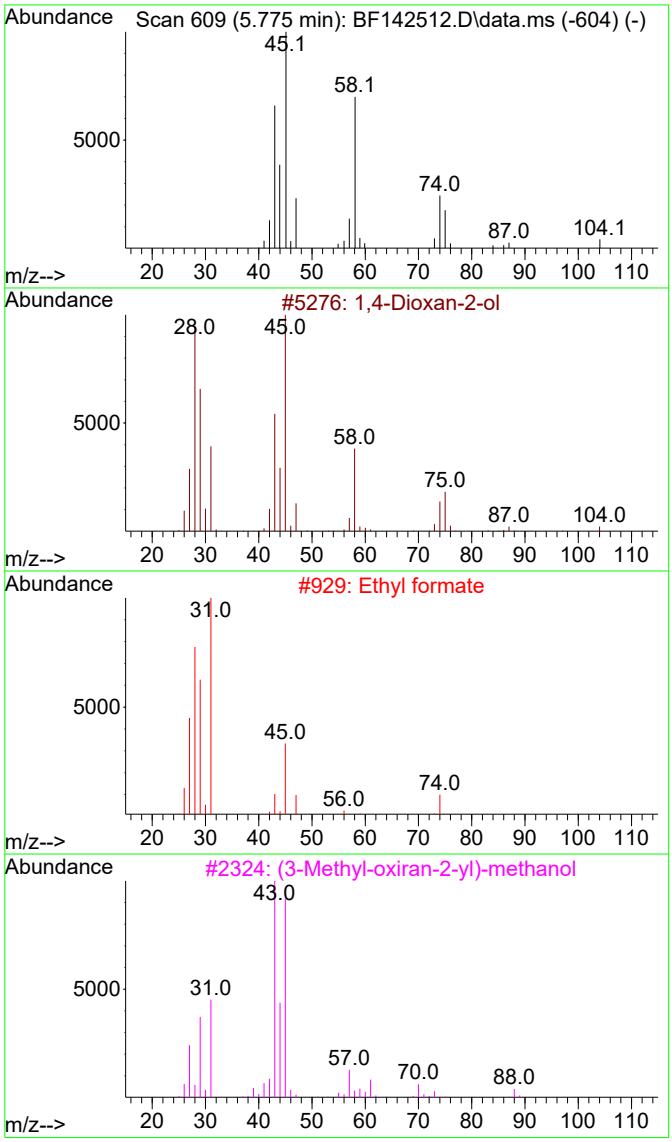
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

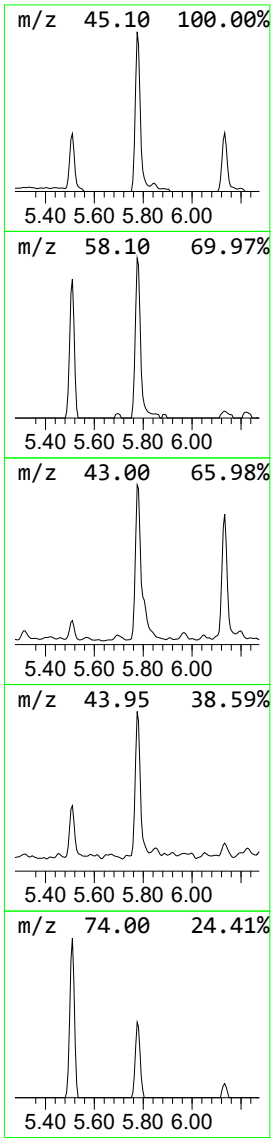
****

Peak Number 3 1,4-Dioxan-2-ol Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.775	2.66 ng	83928	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	64
2	Ethyl formate	74	C3H6O2	000109-94-4	47
3	(3-Methyl-oxiran-2-yl)-methanol	88	C4H8O2	1000194-22-9	38
4	Nitroacetamide	104	C2H4N2O3	014011-21-3	30
5	2-Isopropoxyethylamine	103	C5H13NO	081731-43-3	27





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052225\
Data File : BF142512.D
Acq On : 22 May 2025 16:04
Operator : RC/JU
Sample : Q2052-01
Misc :
ALS Vial : 12 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

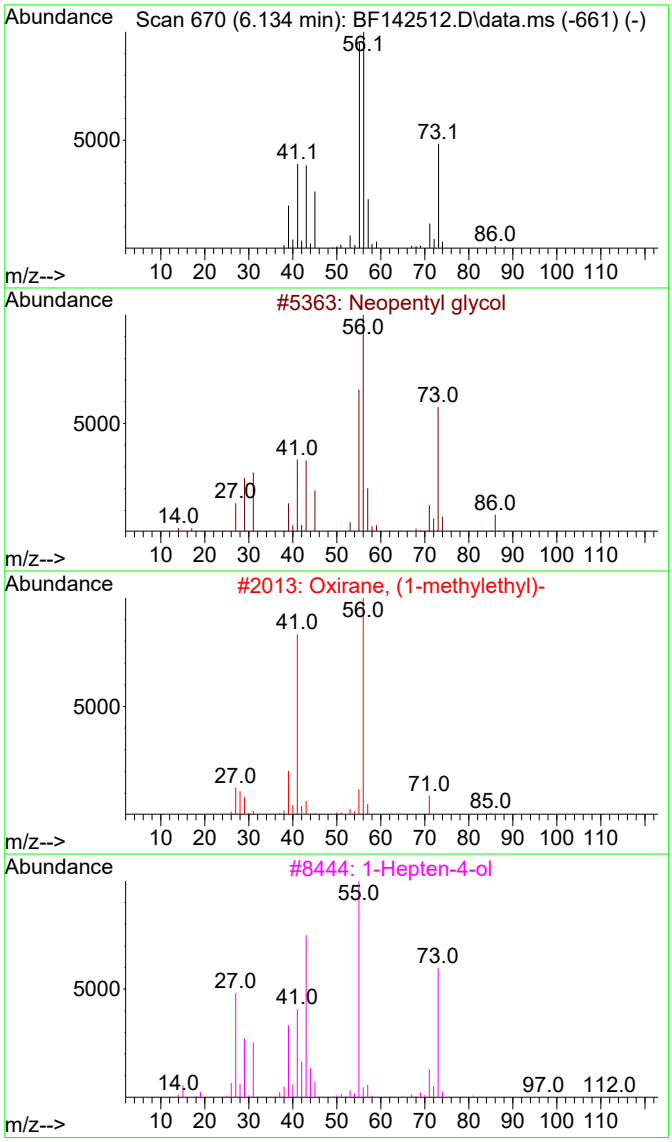
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

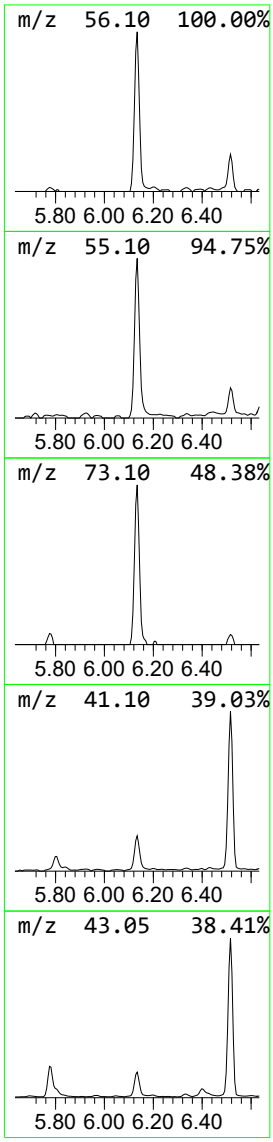
****

Peak Number 4 Neopentyl glycol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.134	3.32 ng	104474	1,4-Dichlorobenzene-d4	6.898

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Neopentyl glycol	104	C5H12O2	000126-30-7	78
2	Oxirane, (1-methylethyl)-	86	C5H10O	001438-14-8	38
3	1-Hepten-4-ol	114	C7H14O	003521-91-3	10
4	2-Propenal	56	C3H4O	000107-02-8	9
5	Ethane, diazo-	56	C2H4N2	001117-96-0	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052225\
Data File : BF142512.D
Acq On : 22 May 2025 16:04
Operator : RC/JU
Sample : Q2052-01
Misc :
ALS Vial : 12 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

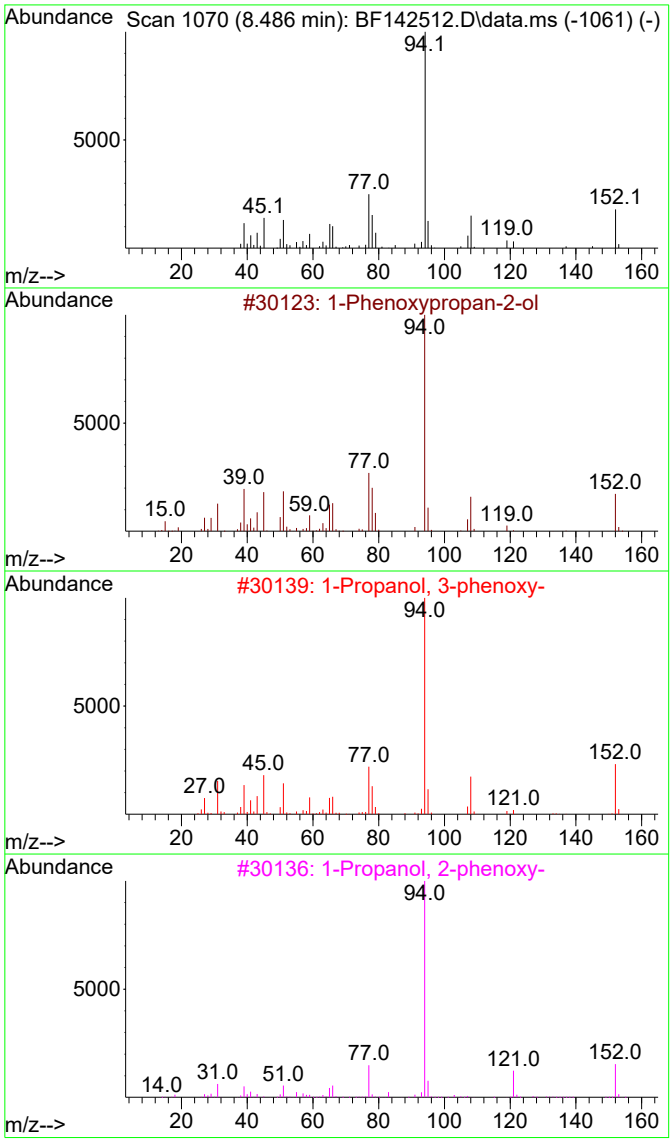
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

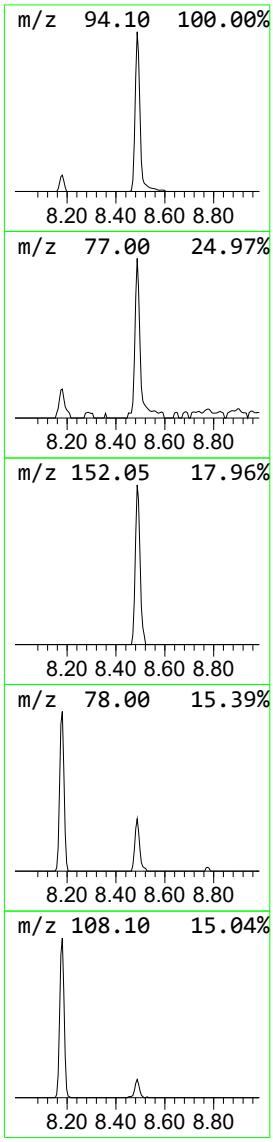
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.486	3.05 ng	114595	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	93
3	1-Propanol, 2-phenoxy-	152	C9H12O2	004169-04-4	64
4	Ethanol, 2-phenoxy-	138	C8H10O2	000122-99-6	64
5	Benzene, (2-methylpropoxy)-	150	C10H14O	001126-75-6	53





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052225\
Data File : BF142512.D
Acq On : 22 May 2025 16:04
Operator : RC/JU
Sample : Q2052-01
Misc :
ALS Vial : 12 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

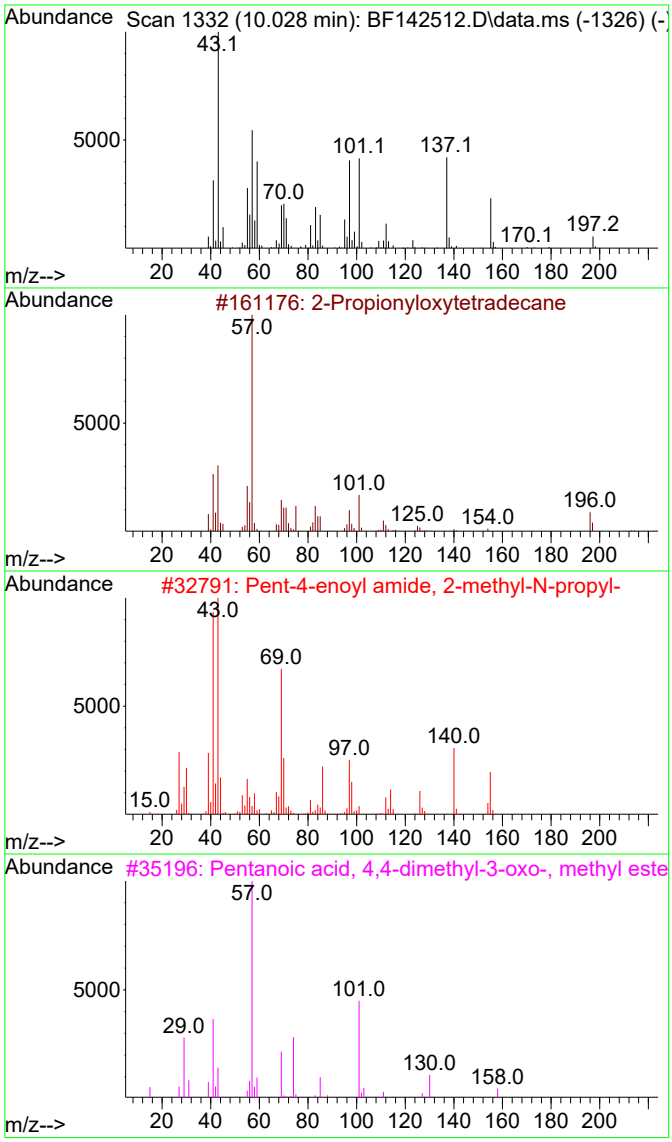
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

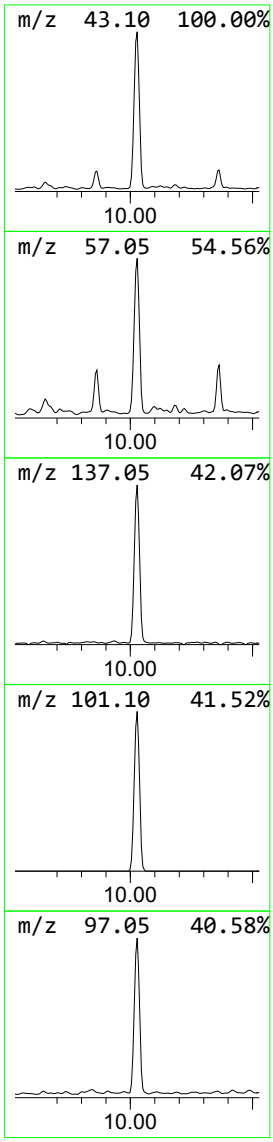
****

Peak Number 6 unknown10.028 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.028	14.04 ng	465086	Acenaphthene-d10	9.933

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propionyloxytetradecane	270	C17H34O2	1000245-62-7	16
2	Pent-4-enoyl amide, 2-methyl-N-p...	155	C9H17NO	1000420-35-2	10
3	Pentanoic acid, 4,4-dimethyl-3-o...	158	C8H14O3	055107-14-7	10
4	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	10
5	6,10,14-Trimethyl-pentadecan-2-ol	270	C18H38O	069729-17-5	10





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052225\
Data File : BF142512.D
Acq On : 22 May 2025 16:04
Operator : RC/JU
Sample : Q2052-01
Misc :
ALS Vial : 12 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

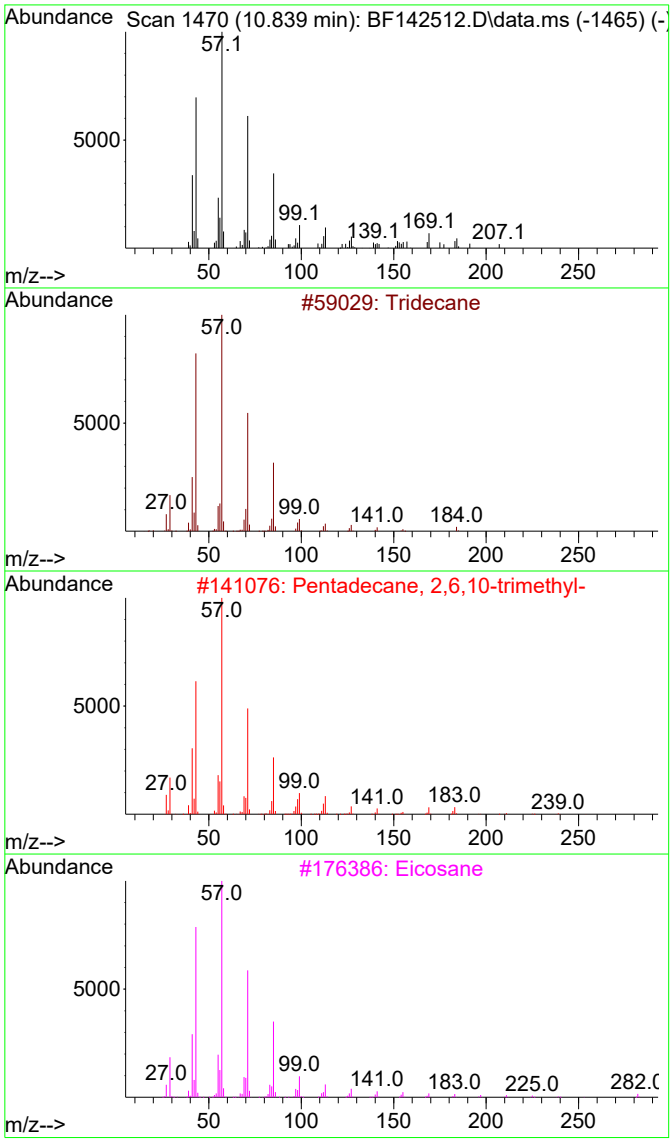
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

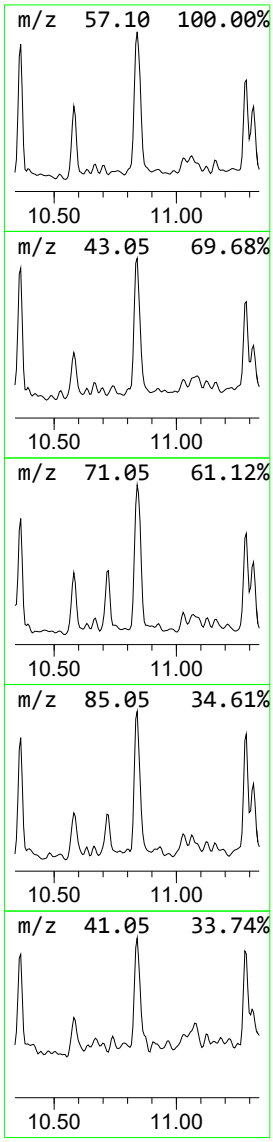
****

Peak Number 7 Tridecane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.839	2.15 ng	76816	Phenanthrene-d10	11.422

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane	184	C13H28	000629-50-5	87
2	Pentadecane, 2,6,10-trimethyl-	254	C18H38	003892-00-0	86
3	Eicosane	282	C20H42	000112-95-8	83
4	Dodecane, 1-iodo-	296	C12H25I	004292-19-7	80
5	Heptacosane	380	C27H56	000593-49-7	80





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052225\
Data File : BF142512.D
Acq On : 22 May 2025 16:04
Operator : RC/JU
Sample : Q2052-01
Misc :
ALS Vial : 12 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

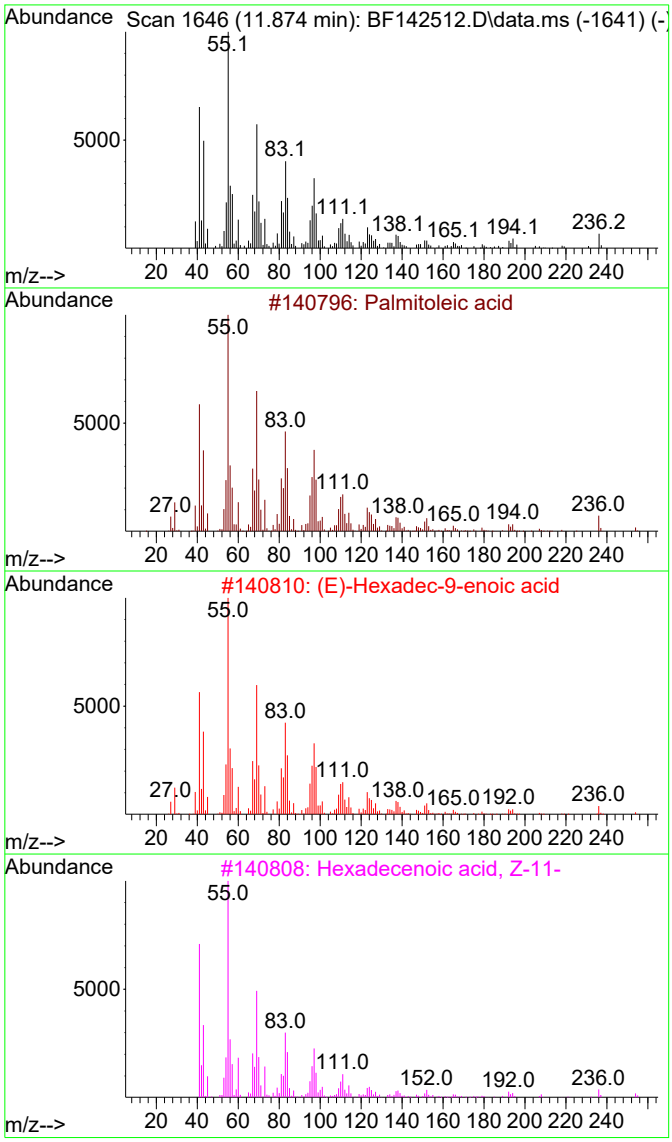
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

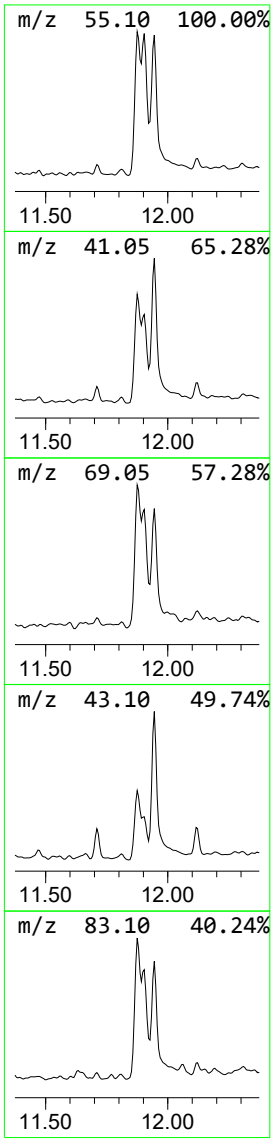
****

Peak Number 8 Palmitoleic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.874	7.02 ng	251452	Phenanthrene-d10	11.422

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Palmitoleic acid	254	C16H30O2	000373-49-9	93
2	(E)-Hexadec-9-enoic acid	254	C16H30O2	010030-73-6	93
3	Hexadecenoic acid, Z-11-	254	C16H30O2	002416-20-8	90
4	cis-2-Methyl-4-n-pentylthiane, S...	218	C11H22O2S	1000215-67-9	76
5	Oxacyclotetradecane-2,11-dione, ...	240	C14H24O3	074685-36-2	68





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Data File : BF142512.D
Acq On : 22 May 2025 16:04
Operator : RC/JU
Sample : Q2052-01
Misc :
ALS Vial : 12 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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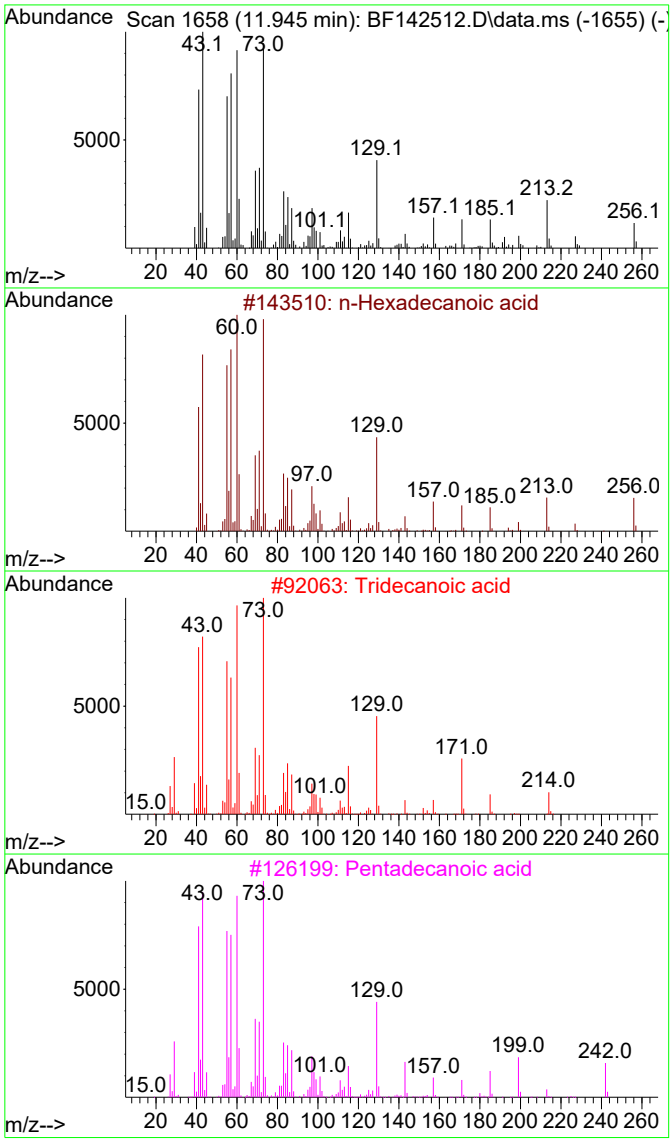
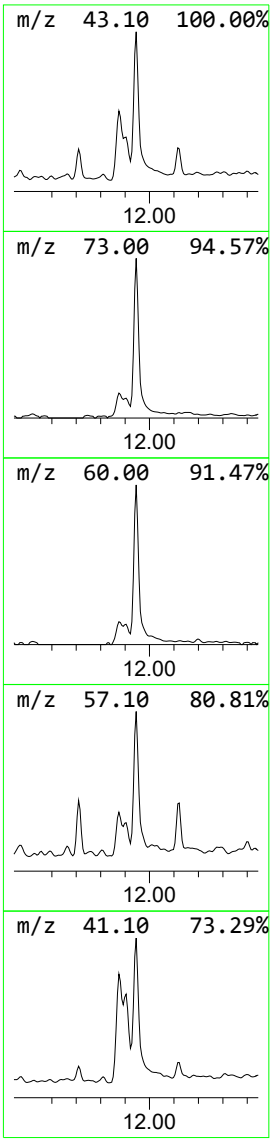
Peak Number 9 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.945	7.70 ng	275617	Phenanthrene-d10	11.422

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	93
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	81
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5	n-Decanoic acid	172	C10H20O2	000334-48-5	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052225\
Data File : BF142512.D
Acq On : 22 May 2025 16:04
Operator : RC/JU
Sample : Q2052-01
Misc :
ALS Vial : 12 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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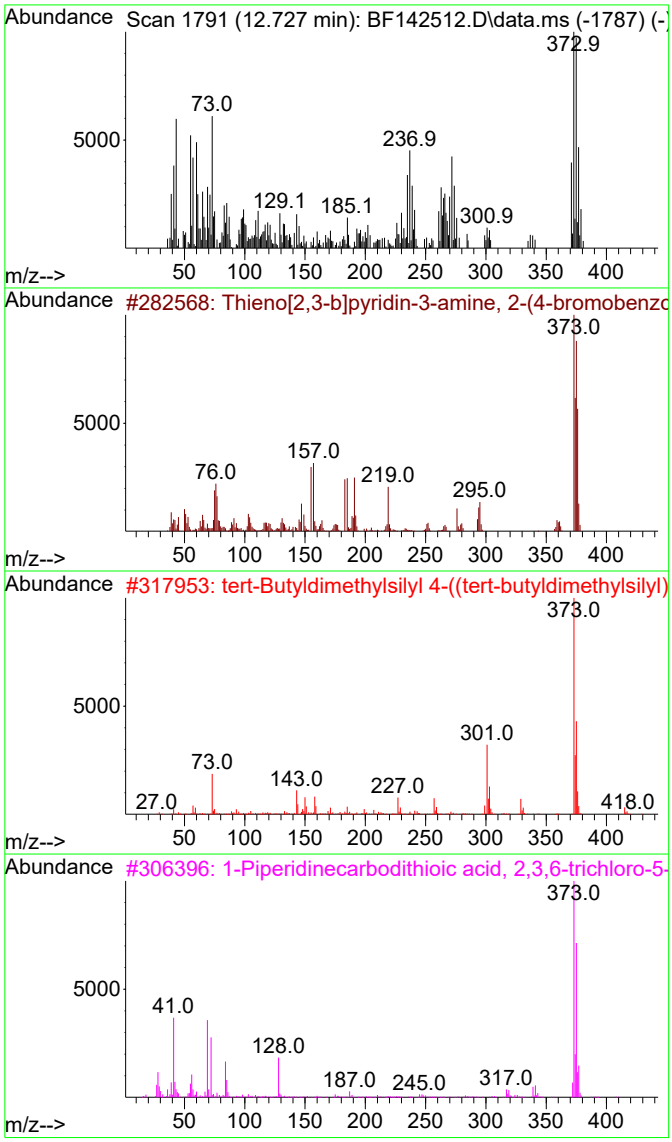
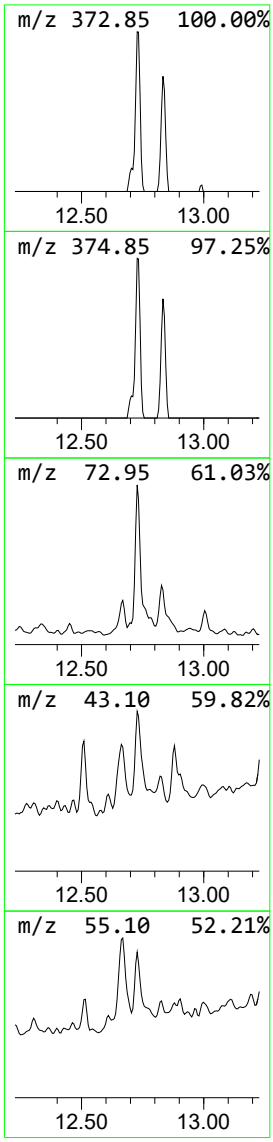
Peak Number 10 unknown12.727 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.727	3.68 ng	131813	Phenanthrene-d10	11.422

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Thieno[2,3-b]pyridin-3-amine, 2-...	374	C17H15BrN2OS	312316-45-3	17
2	tert-Butyldimethylsilyl 4-((tert...	430	C20H35ClO4Si2	1000385-75-1	12
3	1-Piperidinecarbodithioic acid, ...	408	C12H10Cl3F3N2S2	1000305-31-5	12
4	2-(4-Bromo-phenyl)-6-methyl-4-ph...	373	C22H16BrN	071858-09-8	12
5	Quinoline, N-oxy-4-[2-[3-[p-chlo...	373	C23H16ClNO2	1000211-32-6	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052225\
Data File : BF142512.D
Acq On : 22 May 2025 16:04
Operator : RC/JU
Sample : Q2052-01
Misc :
ALS Vial : 12 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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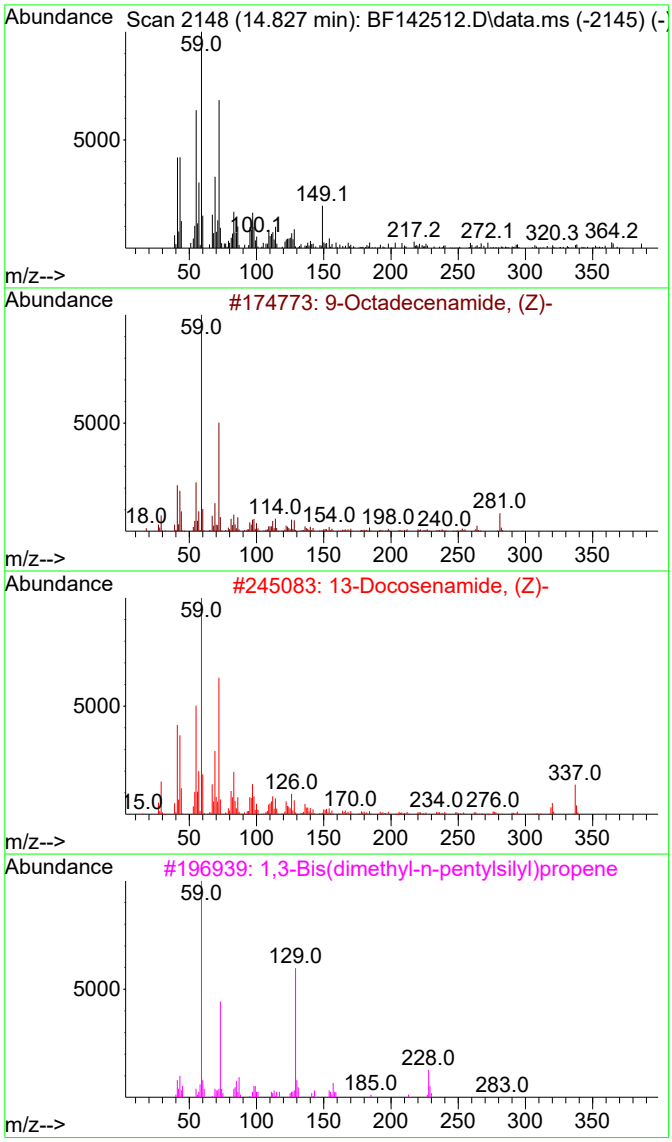
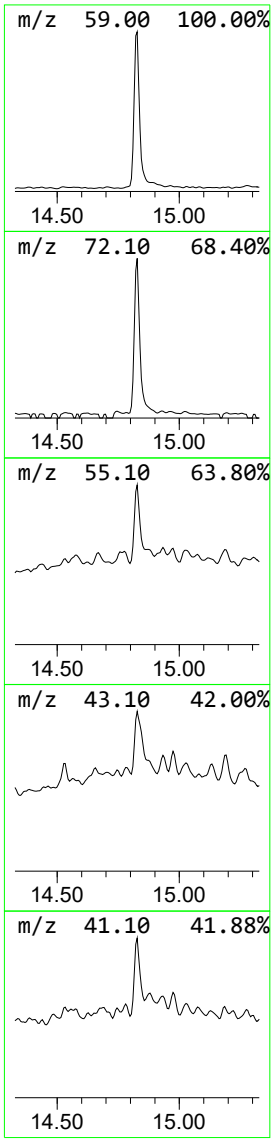
Peak Number 11 9-Octadecenamide, (Z)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.827	4.21 ng	92007	Perylene-d12	15.557

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	80
2	13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	52
3	1,3-Bis(dimethyl-n-pentylsilyl)p...	298	C17H38Si2	136935-56-3	38
4	Palmitoleamide	253	C16H31NO	106010-22-4	38
5	d,l-trans-4-Methyl-5-methoxy-1-(...	184	C11H20O2	1000101-22-2	38





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052225\
Data File : BF142512.D
Acq On : 22 May 2025 16:04
Operator : RC/JU
Sample : Q2052-01
Misc :
ALS Vial : 12 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
Propylene Glycol	3.404	6.5	ng	204644	1	6.898	629870	20.0
2-Pentanone, 4-...	5.104	5.8	ng	183703	1	6.898	629870	20.0
1,4-Dioxan-2-ol	5.775	2.7	ng	83928	1	6.898	629870	20.0
Neopentyl glycol	6.134	3.3	ng	104474	1	6.898	629870	20.0
1-Phenoxypropan...	8.486	3.0	ng	114595	2	8.181	751177	20.0
unknown10.028	10.028	14.0	ng	465086	3	9.933	662754	20.0
Tridecane	10.839	2.1	ng	76816	4	11.422	716064	20.0
Palmitoleic acid	11.874	7.0	ng	251452	4	11.422	716064	20.0
n-Hexadecanoic ...	11.945	7.7	ng	275617	4	11.422	716064	20.0
unknown12.727	12.727	3.7	ng	131813	4	11.422	716064	20.0
9-Octadecenamid...	14.827	4.2	ng	92007	6	15.557	437076	20.0