LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF031425\
Data File : BF141961.D
Acq On : 14 Mar 2025 13:11
Operator : RC/JU
Sample : Q1566-01 5X
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CTWK-COMP

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-BF031025.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF141961.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.134	3	7	15	rVB	277073	437440	36.98%	3.107%
2	2.252	22	27	43	rVB	7195	18805	1.59%	0.134%
3	5.081	501	508	514	rBV2	7118	12743	1.08%	0.090%
4	5.481	571	576	591	rBV	537052	704926	59.59%	5.006%
5	6.487	742	747	759	rBV	562210	739382	62.50%	5.251%
6	6.875	808	813	820	rBV	603433	746622	63.12%	5.302%
7	7.434	902	908	918	rBV	353706	481970	40.74%	3.423%
8	7.687	947	951	959	rBV	14654	20040	1.69%	0.142%
9	8.157	1025	1031	1052	rBV	784778	1002846	84.78%	7.122%
10	9.228	1208	1213	1223	rBV	862456	1066231	90.13%	7.572%
11	9.769	1301	1305	1312	rBV	10161	17751	1.50%	0.126%
12	9.910	1323	1329	1334	rBV	937789	1172367	99.11%	8.326%
13	10.098	1356	1361	1373	rVB4	26074	49547	4.19%	0.352%
14	10.622	1445	1450	1457	rVB	211701	271853	22.98%	1.931%
15	10.692	1457	1462	1474	rBV	529515	676931	57.22%	4.807%
16	10.822	1479	1484	1490	rVB5	9660	16289	1.38%	0.116%
17	10.928	1498	1502	1507	rBV	27380	35127	2.97%	0.249%
18	11.051	1517	1523	1530	rBV3	20405	36040	3.05%	0.256%
19	11.392	1576	1581	1589	rBV	879947	1182932	100.00%	8.401%
20	11.628	1615	1621	1628	rBV8	17478	47863	4.05%	0.340%
21	11.845	1653	1658	1662	rBV7	9427	19467	1.65%	0.138%
22	11.916	1663	1670	1682	rBV	465792	808508	68.35%	5.742%
23	12.004	1682	1685	1688	rVV2	9547	13466	1.14%	0.096%
24	12.169	1708	1713	1719	rBV2	85862	126865	10.72%	0.901%
25	12.445	1757	1760	1763	rBV3	18880	24801	2.10%	0.176%
26	12.604	1783	1787	1796	rBV	48355	96111	8.12%	0.683%
27	12.704	1798	1804	1817	rVV	179780	324114	27.40%	2.302%
28	12.833	1822	1826	1832	rBV	63319	91037	7.70%	0.647%
29	12.975	1845	1850	1859	rVB	752832	961520	81.28%	6.828%
30	13.051	1860	1863	1870	rVB3	11780	19956	1.69%	0.142%
31	13.145	1875	1879	1885	rVB	12199	27211	2.30%	0.193%
32	13.210	1886	1890	1895	rVV2	14250	22894	1.94%	0.163%
33	13.269	1896	1900	1907	rVB2	12739	23313	1.97%	0.166%
34	13.545	1942	1947	1956	rVB3	21309	47055	3.98%	0.334%
35	13.669	1965	1968	1973	rVB	12253	16730	1.41%	0.119%
36	13.880	1999	2004	2013	rBV	47855	84978	7.18%	0.603%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF031425\
Data File : BF141961.D
Acq On : 14 Mar 2025 13:11
Operator : RC/JU
Sample : Q1566-01 5X
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CTWK-COMP

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-BF031025.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	14.027	2023	2029	2041	rBV	570968	826305	69.85%	5.868%
38	14.192	2054	2057	2063	rVB	29878	43816	3.70%	0.311%
39	14.422	2091	2096	2099	rBV2	23047	38335	3.24%	0.272%
40	14.498	2105	2109	2113	rBV	43322	66019	5.58%	0.469%
41	14.551	2114	2118	2124	rVB3	40824	67265	5.69%	0.478%
42	14.669	2134	2138	2146	rVB5	13485	29162	2.47%	0.207%
43	14.810	2158	2162	2165	rBV	27358	38219	3.23%	0.271%
44	14.880	2171	2174	2182	rVB	43240	70908	5.99%	0.504%
45	15.069	2201	2206	2214	rBV2	27212	64397	5.44%	0.457%
46	15.151	2215	2220	2230	rVB	90971	148001	12.51%	1.051%
47	15.368	2252	2257	2262	rVB2	25414	48724	4.12%	0.346%
48	15.427	2263	2267	2273	rVV	26222	50507	4.27%	0.359%
49	15.498	2273	2279	2294	rVB	513434	859635	72.67%	6.105%
50	15.980	2355	2361	2367	rBV	62641	111589	9.43%	0.792%
51	16.415	2429	2435	2443	rBV	60675	117805	9.96%	0.837%
52	16.980	2525	2531	2538	rBV3	17629	54851	4.64%	0.390%

Sum of corrected areas: 14081269

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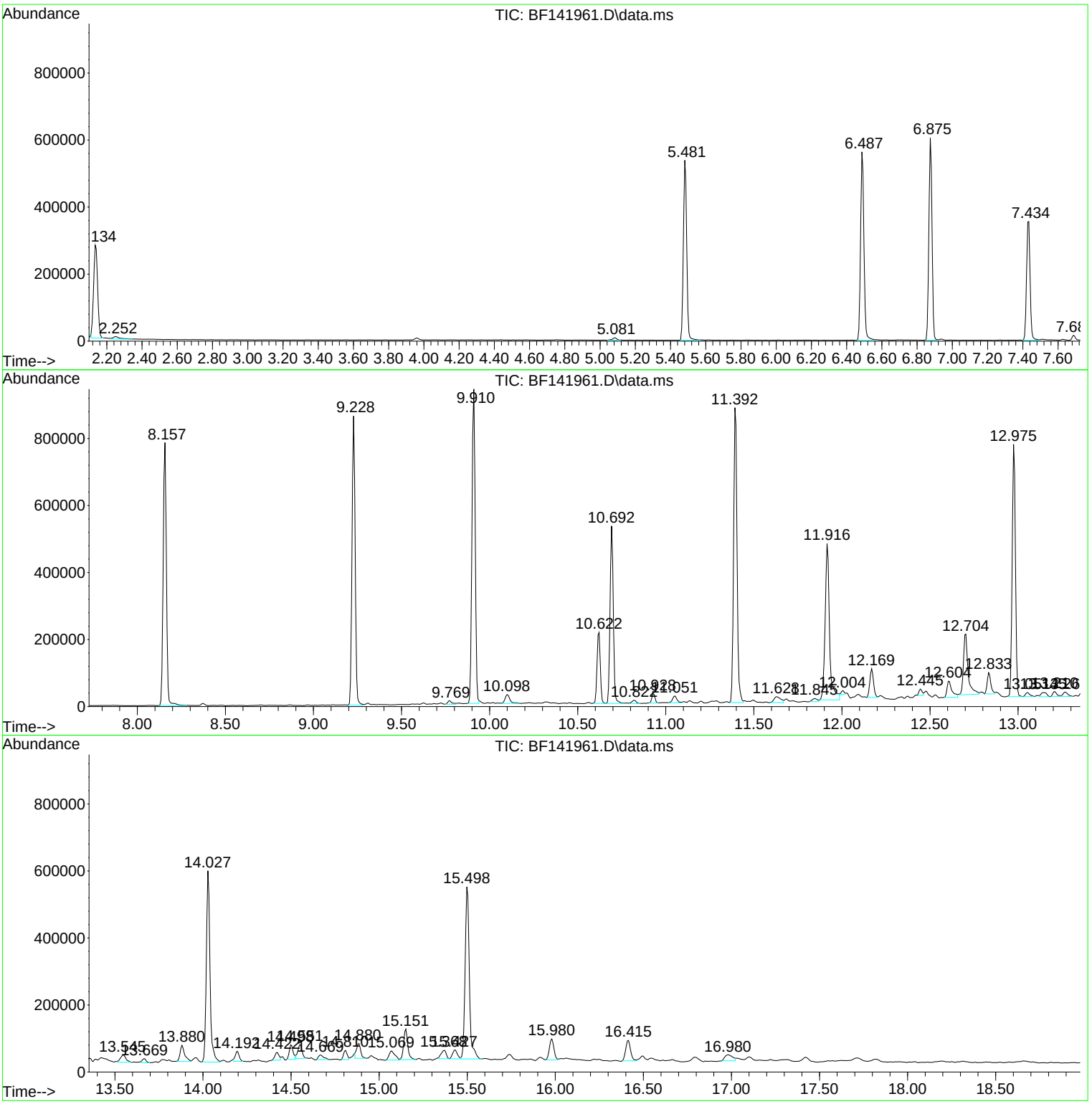
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CTWK-COMP

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF031025.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\BF031425\
Data File : BF141961.D
Acq On : 14 Mar 2025 13:11
Operator : RC/JU
Sample : Q1566-01 5X
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CTWK-COMP

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF031025.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

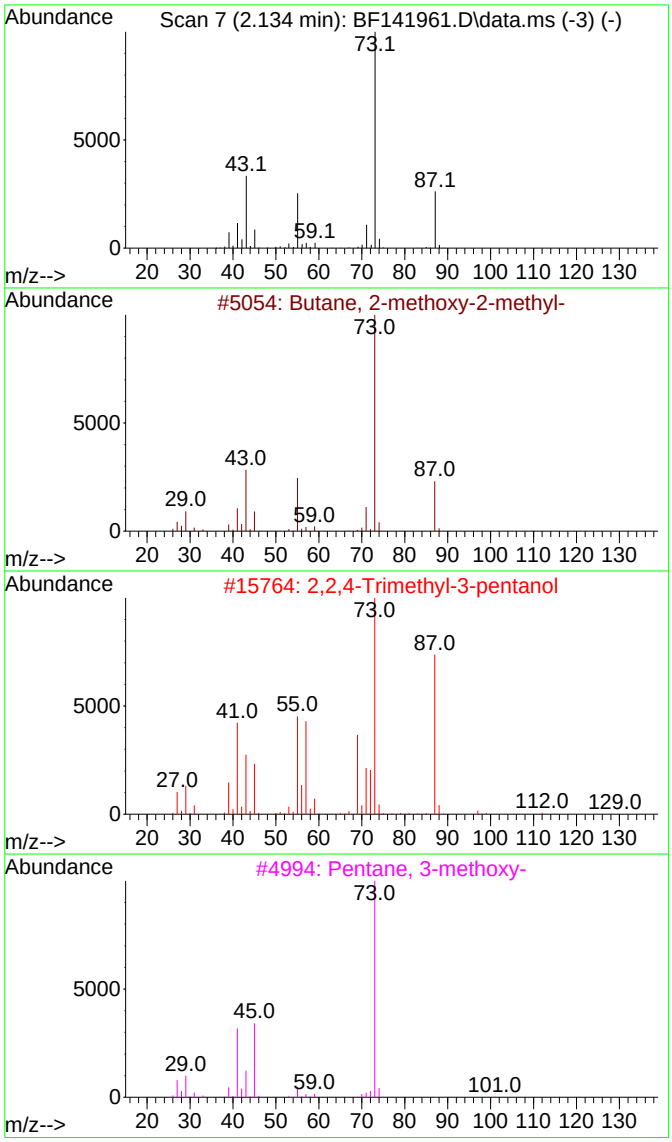
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

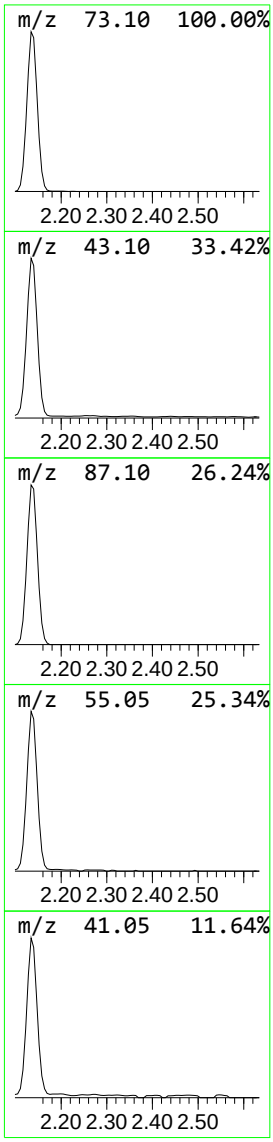
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.134	11.72 ng	437440	1,4-Dichlorobenzene-d4	6.875

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
4	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	22
5	Silane, tetramethyl-	88	C4H12Si	000075-76-3	17





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF031425\
Data File : BF141961.D
Acq On : 14 Mar 2025 13:11
Operator : RC/JU
Sample : Q1566-01 5X
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CTWK-COMP

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF031025.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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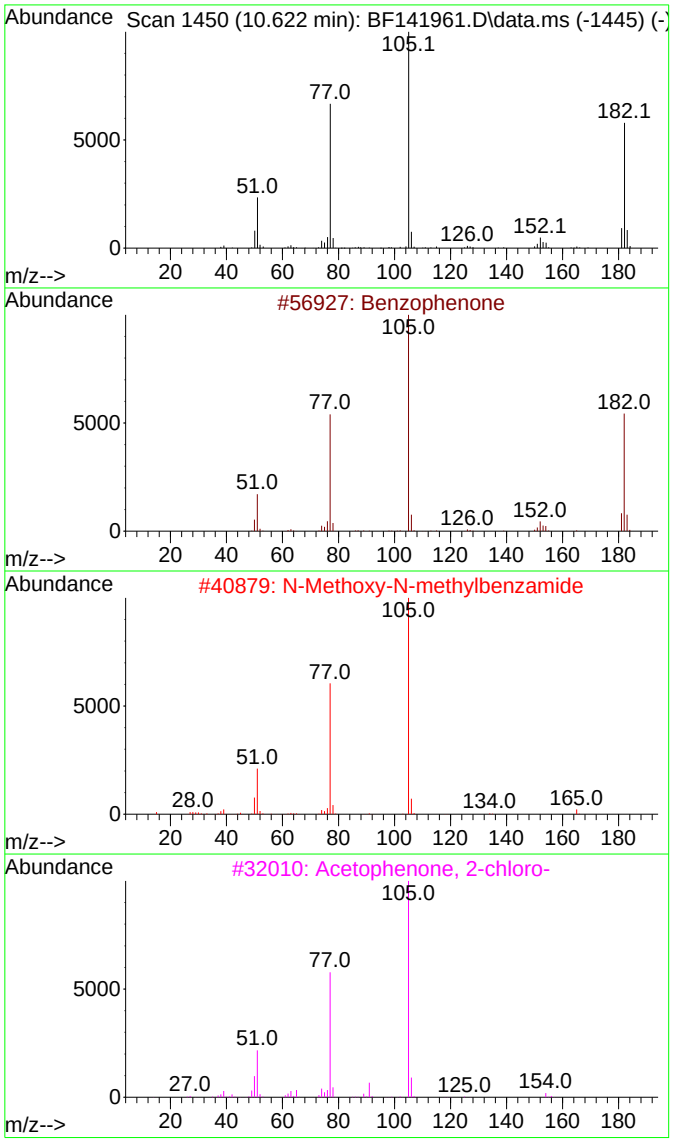
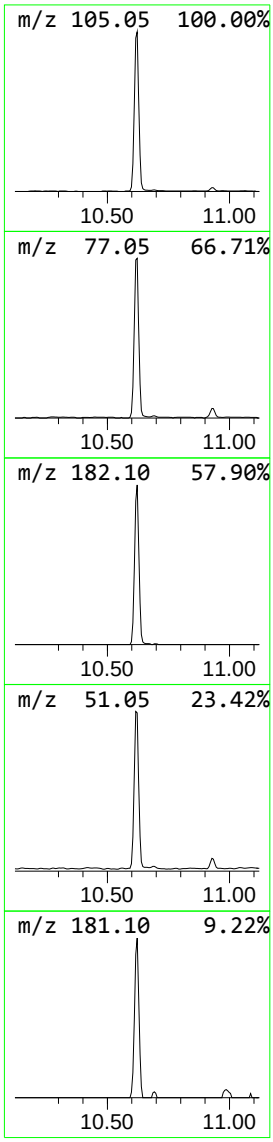
Peak Number 2 Benzophenone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.622	4.64 ng	271853	Acenaphthene-d10	9.910

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	N-Methoxy-N-methylbenzamide	165	C9H11NO2	006919-61-5	49
3	Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	49
4	1,2-Propanedione, 1-phenyl-	148	C9H8O2	000579-07-7	47
5	Vinyl benzoate	148	C9H8O2	000769-78-8	47





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF031425\
Data File : BF141961.D
Acq On : 14 Mar 2025 13:11
Operator : RC/JU
Sample : Q1566-01 5X
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CTWK-COMP

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF031025.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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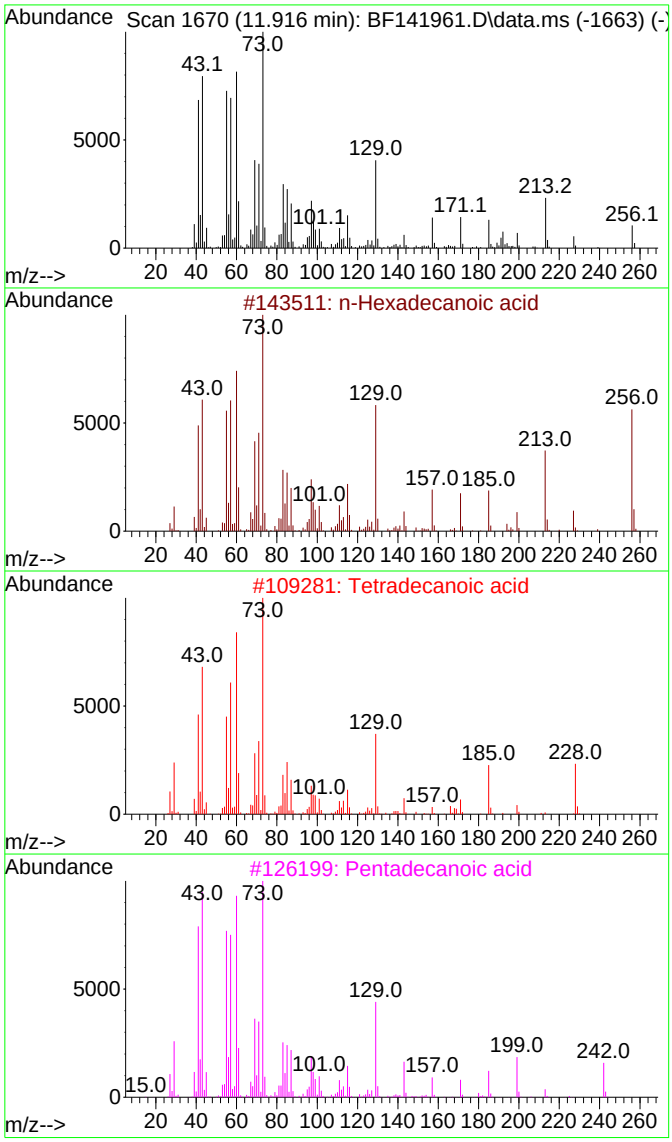
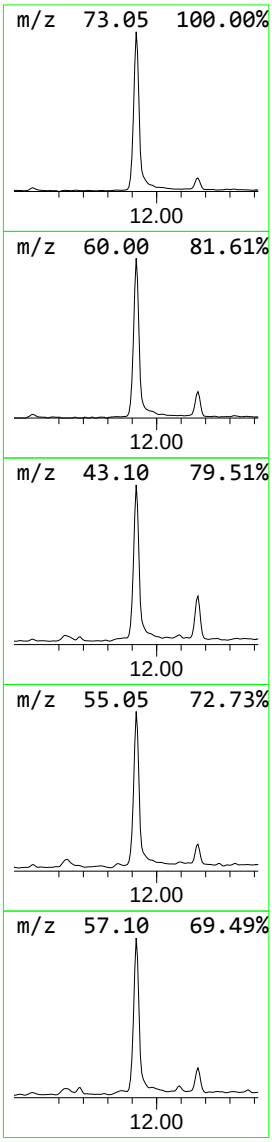
Peak Number 3 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.916	13.67 ng	808508	Phenanthrene-d10	11.392

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	94
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
4	Tridecanoic acid	214	C13H26O2	000638-53-9	91
5	n-Decanoic acid	172	C10H20O2	000334-48-5	68





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF031425\
Data File : BF141961.D
Acq On : 14 Mar 2025 13:11
Operator : RC/JU
Sample : Q1566-01 5X
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CTWK-COMP

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF031025.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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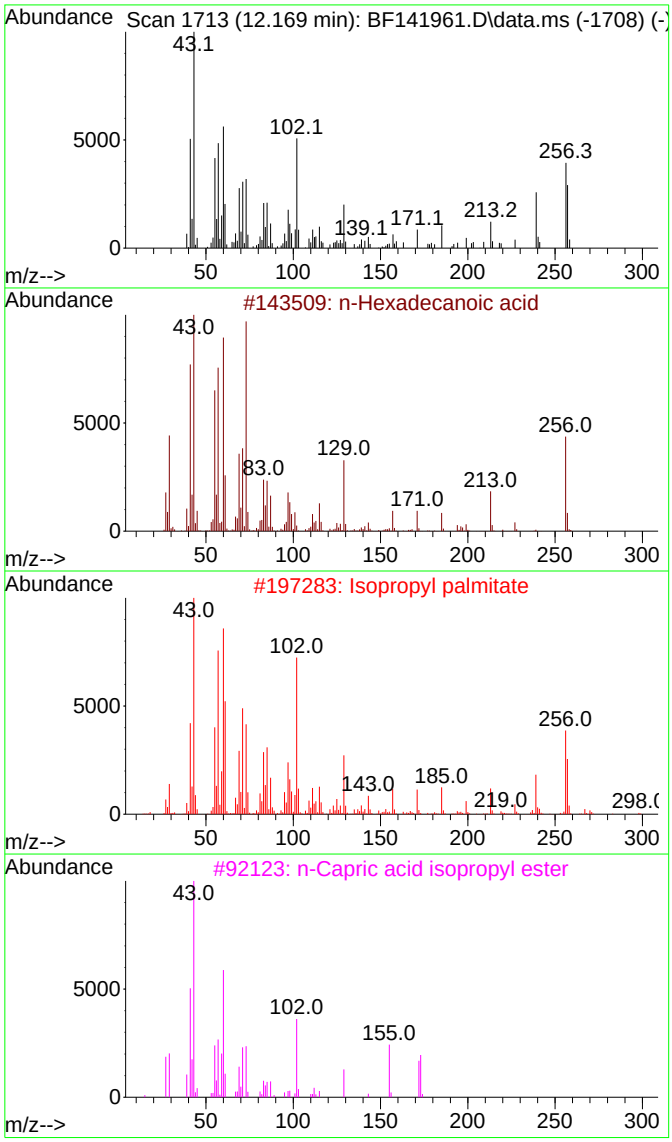
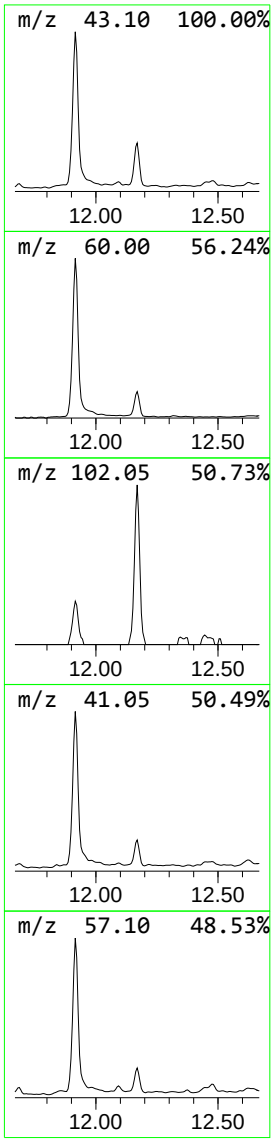
Peak Number 4 Isopropyl palmitate Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.169	2.14 ng	126865	Phenanthrene-d10	11.392

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	91
2	Isopropyl palmitate	298	C19H38O2	000142-91-6	74
3	n-Capric acid isopropyl ester	214	C13H26O2	002311-59-3	38
4	Octanoic acid	144	C8H16O2	000124-07-2	11
5	(S)-2-Allyl-3-benzyl-7-fluoro-3,...	347	C18H18FNO3S	1000481-48-6	10





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF031425\
Data File : BF141961.D
Acq On : 14 Mar 2025 13:11
Operator : RC/JU
Sample : Q1566-01 5X
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CTWK-COMP

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF031025.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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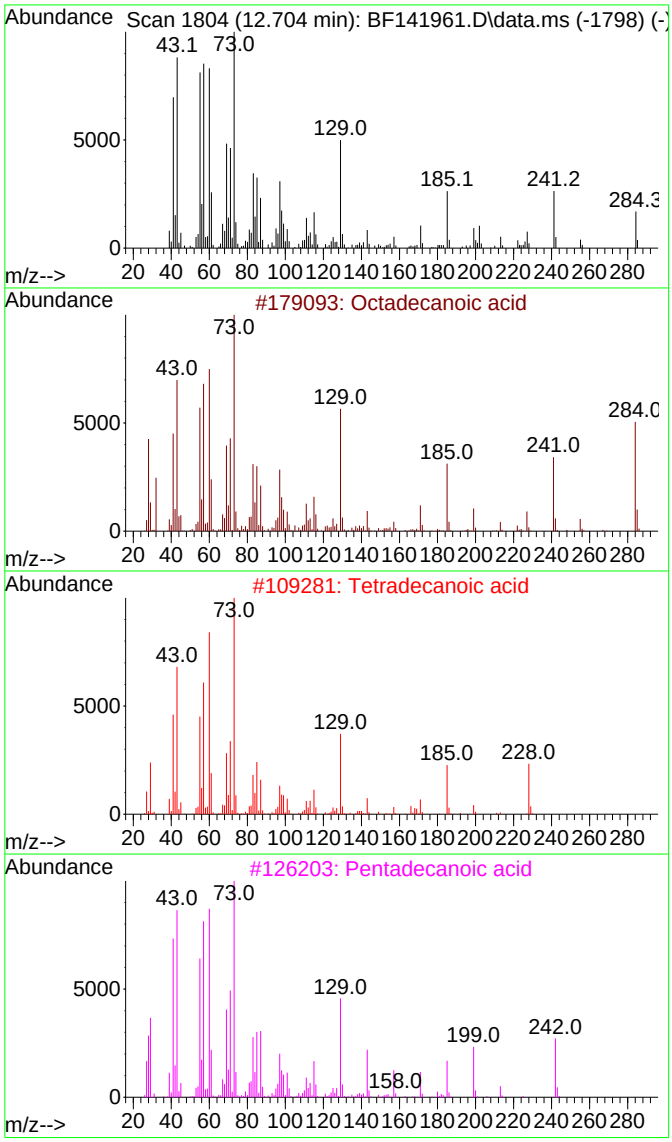
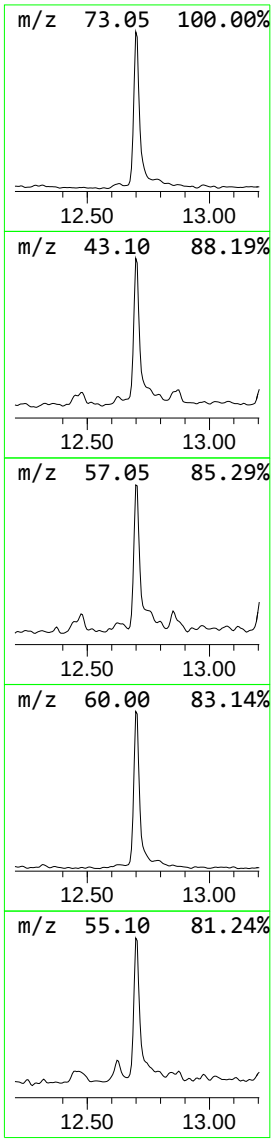
Peak Number 5 Octadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.704	5.48 ng	324114	Phenanthrene-d10	11.392

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	83
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	81
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	80
5	Tridecanoic acid	214	C13H26O2	000638-53-9	72





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF031425\
Data File : BF141961.D
Acq On : 14 Mar 2025 13:11
Operator : RC/JU
Sample : Q1566-01 5X
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF031025.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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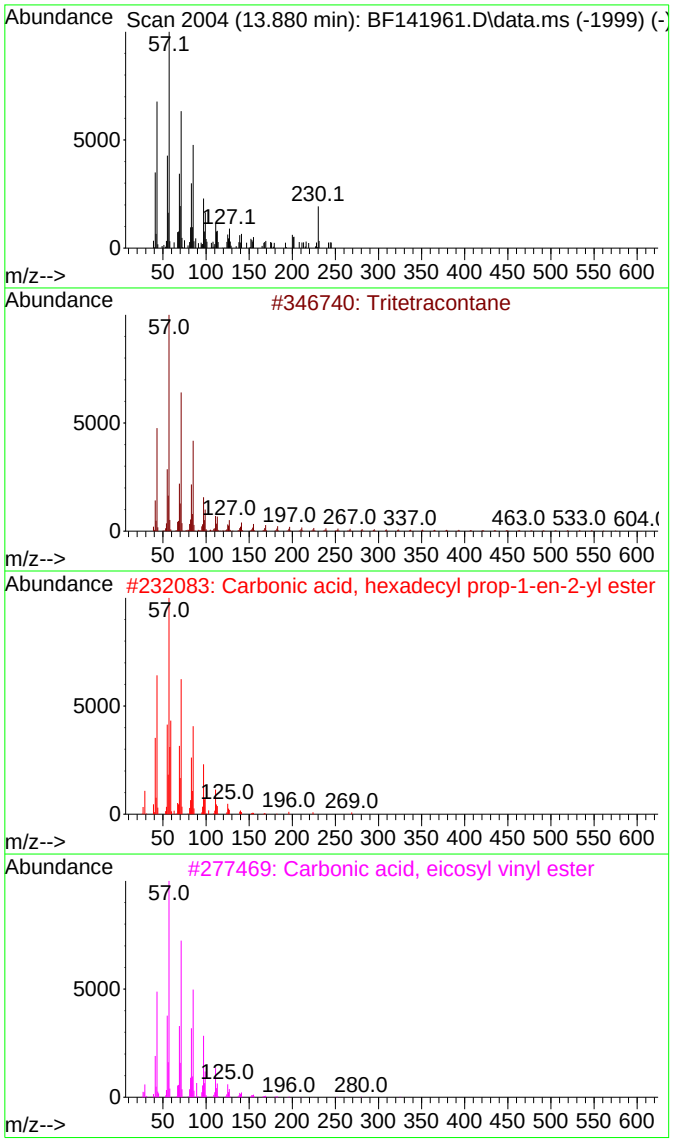
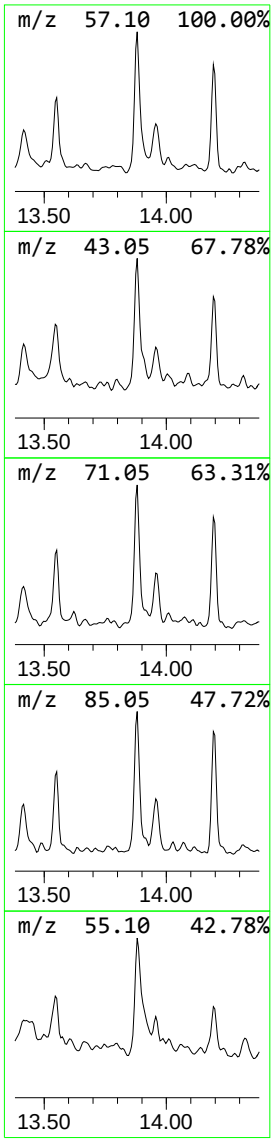
Peak Number 7 Tritetracontane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.880	2.06 ng	84978	Chrysene-d12	14.027

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tritetracontane	605	C43H88	007098-21-7	80
2	Carbonic acid, hexadecyl prop-1-...	326	C20H38O3	1000382-90-3	74
3	Carbonic acid, eicosyl vinyl ester	368	C23H44O3	1000382-54-3	74
4	Sulfurous acid, butyl heptadecyl...	376	C21H44O3S	1000309-18-4	74
5	Carbonic acid, octadecyl prop-1-...	354	C22H42O3	1000383-11-5	74





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF031425\
Data File : BF141961.D
Acq On : 14 Mar 2025 13:11
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Sample : Q1566-01 5X
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CTWK-COMP

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF031025.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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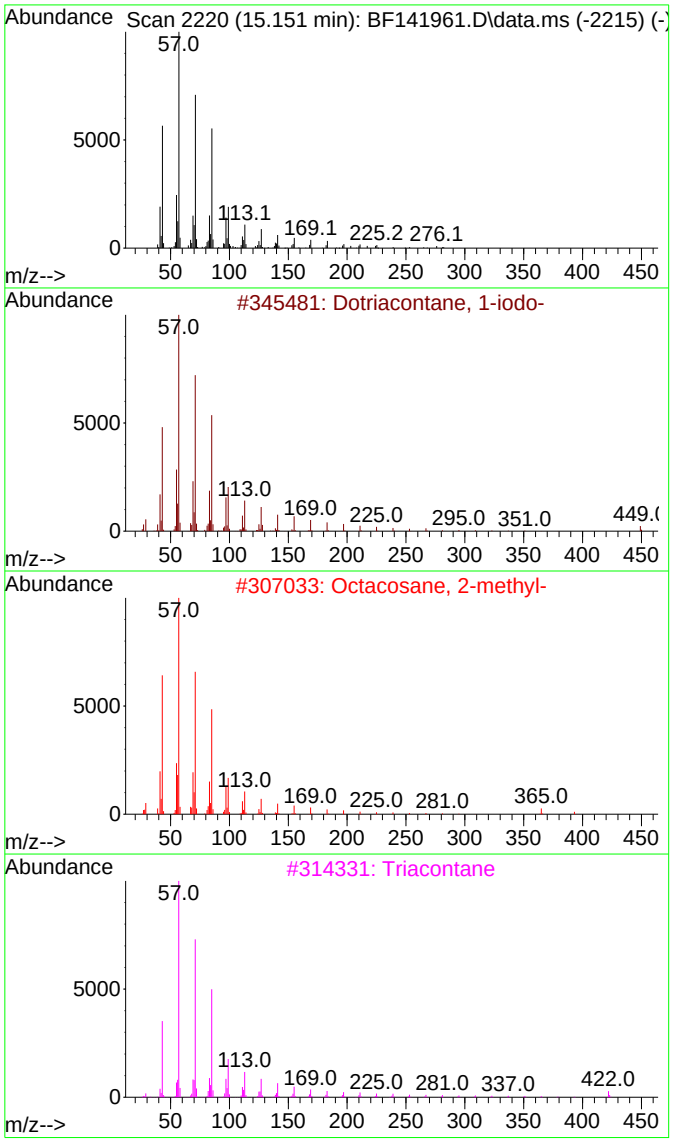
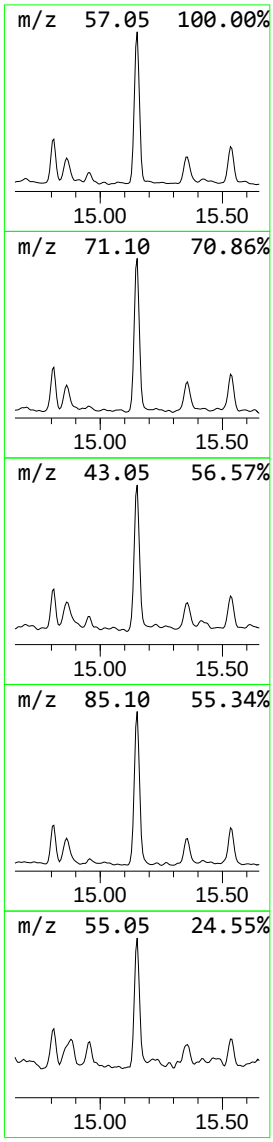
Peak Number 8 Dotriacontane, 1-iodo- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.151	3.44 ng	148001	Perylene-d12	15.498

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dotriacontane, 1-iodo-	576	C32H65I	1000406-32-4	91
2	Octacosane, 2-methyl-	408	C29H60	001560-98-1	91
3	Triacontane	422	C30H62	000638-68-6	91
4	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
5	Heneicosane	296	C21H44	000629-94-7	90





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF031425\
Data File : BF141961.D
Acq On : 14 Mar 2025 13:11
Operator : RC/JU
Sample : Q1566-01 5X
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CTWK-COMP

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF031025.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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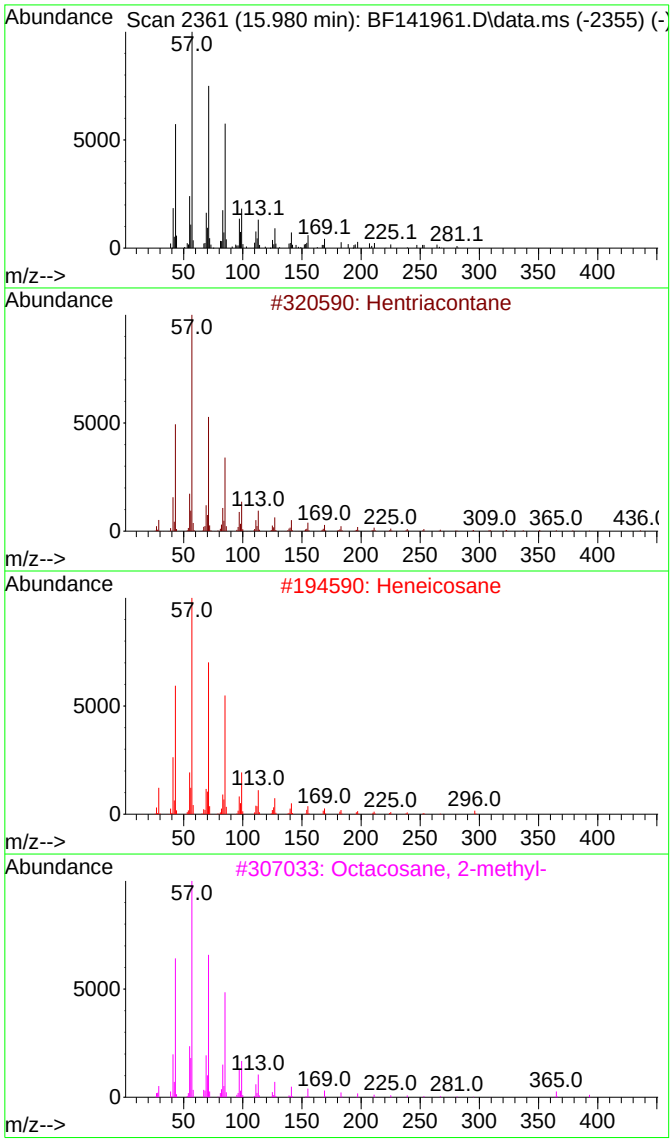
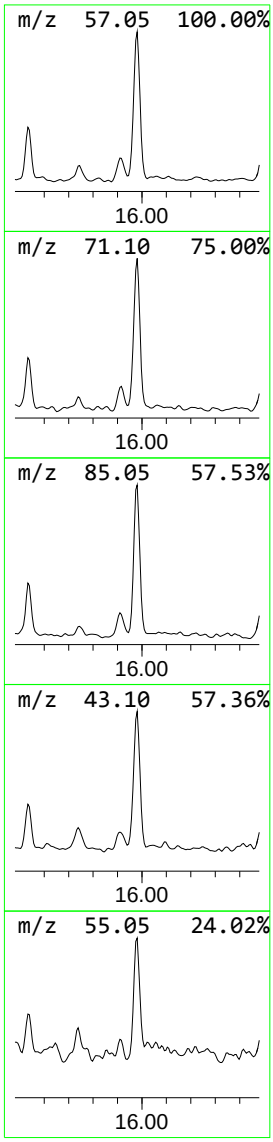
Peak Number 9 Hentriacontane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.980	2.60 ng	111589	Perylene-d12	15.498

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hentriacontane	437	C31H64	000630-04-6	91
2	Heneicosane	296	C21H44	000629-94-7	91
3	Octacosane, 2-methyl-	408	C29H60	001560-98-1	91
4	Heptacosane	380	C27H56	000593-49-7	91
5	Dotriacontane, 1-iodo-	576	C32H65I	1000406-32-4	91





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF031425\
Data File : BF141961.D
Acq On : 14 Mar 2025 13:11
Operator : RC/JU
Sample : Q1566-01 5X
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CTWK-COMP

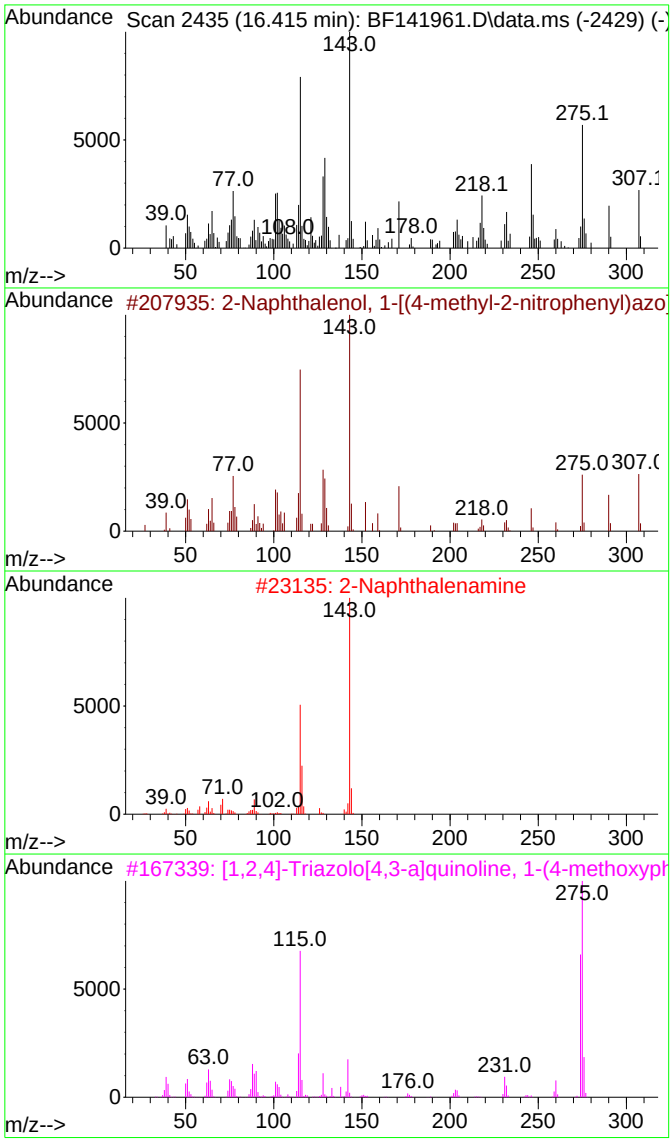
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF031025.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

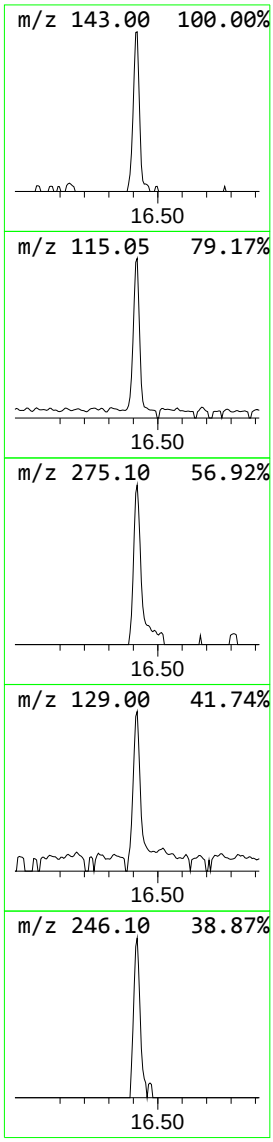
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 2-Naphthalenol, 1-[(4-methy... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.416	2.74 ng	117805	Perylene-d12	15.498

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Naphthalenol, 1-[(4-methyl-2-n...	307	C17H13N3O3	002425-85-6	99
2	2-Naphthalenamine	143	C10H9N	000091-59-8	41
3	[1,2,4]-Triazolo[4,3-a]quinoline...	275	C17H13N3O	002693-40-5	38
4	1H-Pyrrole, 1-phenyl-	143	C10H9N	000635-90-5	38
5	1-Phenyl-1-cyclopropanecarbonitrile	143	C10H9N	000935-44-4	38





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF031425\
Data File : BF141961.D
Acq On : 14 Mar 2025 13:11
Operator : RC/JU
Sample : Q1566-01 5X
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CTWK-COMP

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF031025.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...	2.134	11.7	ng	437440	1	6.875	746622	20.0
Benzophenone	10.622	4.6	ng	271853	3	9.910	1172370	20.0
n-Hexadecanoic ...	11.916	13.7	ng	808508	4	11.392	1182930	20.0
Isopropyl palmi...	12.169	2.1	ng	126865	4	11.392	1182930	20.0
Octadecanoic acid	12.704	5.5	ng	324114	4	11.392	1182930	20.0
Tritetracontane	13.880	2.1	ng	84978	5	14.027	826305	20.0
Dotriacontane, ...	15.151	3.4	ng	148001	6	15.498	859635	20.0
Hentriacontane	15.980	2.6	ng	111589	6	15.498	859635	20.0
2-Naphthalenol,...	16.416	2.7	ng	117805	6	15.498	859635	20.0