LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP092525\
Data File : BP025864.D
Acq On : 25 Sep 2025 19:32
Operator : CG/JU
Sample : Q3168-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TOTES COMP#1

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_P\Methods\8270E-BP091225.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP025864.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.014	8	13	21	rVV	4036692	6440018	77.06%	10.085%
2	3.079	21	24	37	rVB	346043	645314	7.72%	1.011%
3	3.614	110	115	125	rVB2	121328	223850	2.68%	0.351%
4	4.202	209	215	225	rVB2	347002	646803	7.74%	1.013%
5	4.361	234	242	251	rVB6	80586	234412	2.81%	0.367%
6	4.731	294	305	312	rBV	97212	230481	2.76%	0.361%
7	5.002	342	351	361	rVB6	94196	220513	2.64%	0.345%
8	5.102	361	368	372	rBV	261734	410593	4.91%	0.643%
9	5.390	411	417	431	rVB	1427429	2412446	28.87%	3.778%
10	5.637	454	459	463	rBV	383671	564490	6.75%	0.884%
11	5.837	483	493	505	rVB2	402377	840858	10.06%	1.317%
12	6.337	569	578	580	rBV4	88144	219142	2.62%	0.343%
13	6.384	581	586	591	rVB2	206563	415057	4.97%	0.650%
14	6.643	618	630	635	rBV	652118	1177801	14.09%	1.844%
15	6.755	642	649	654	rBV	435947	750540	8.98%	1.175%
16	6.867	658	668	670	rBV5	226905	552601	6.61%	0.865%
17	6.961	678	684	695	rVB	747568	1411727	16.89%	2.211%
18	7.131	706	713	722	rVB2	271520	570453	6.83%	0.893%
19	7.214	722	727	742	rVB	236303	545090	6.52%	0.854%
20	7.578	784	789	798	rVB4	95327	216511	2.59%	0.339%
21	7.755	806	819	825	rBV3	908600	1999848	23.93%	3.132%
22	7.819	825	830	834	rVV	136372	285348	3.41%	0.447%
23	7.884	834	841	845	rVB	311703	600513	7.19%	0.940%
24	8.037	857	867	878	rBV3	290093	698228	8.36%	1.093%
25	8.137	879	884	888	rBV2	174966	300598	3.60%	0.471%
26	8.343	911	919	923	rVB2	139098	292600	3.50%	0.458%
27	8.443	923	936	940	rBV	534158	1506696	18.03%	2.359%
28	8.566	947	957	963	rVB6	263911	729843	8.73%	1.143%
29	8.819	995	1000	1006	rBV	178793	318486	3.81%	0.499%
30	8.902	1006	1014	1020	rBV	1858299	3467057	41.49%	5.429%
31	9.090	1037	1046	1051	rBV	177103	405570	4.85%	0.635%
32	9.319	1080	1085	1090	rBV4	128718	229346	2.74%	0.359%
33	9.396	1091	1098	1102	rBV2	293862	548830	6.57%	0.859%
34	9.508	1111	1117	1121	rBV	245805	410773	4.92%	0.643%
35	9.943	1180	1191	1197	rBV2	661205	1811137	21.67%	2.836%
36	10.108	1210	1219	1229	rBV7	253664	790610	9.46%	1.238%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP092525\
Data File : BP025864.D
Acq On : 25 Sep 2025 19:32
Operator : CG/JU
Sample : Q3168-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TOTES COMP#1

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_P\Methods\8270E-BP091225.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	10.208	1230	1236	1237	rBV	186078	307895	3.68%	0.482%
38	10.308	1247	1253	1258	rVB3	176460	320496	3.84%	0.502%
39	10.372	1260	1264	1272	rVV4	123574	259754	3.11%	0.407%
40	10.519	1279	1289	1297	rBV2	963737	2238826	26.79%	3.506%
41	10.643	1306	1310	1313	rBV3	140385	208269	2.49%	0.326%
42	10.802	1333	1337	1342	rBV2	182864	296544	3.55%	0.464%
43	11.378	1425	1435	1438	rBV6	473325	1331986	15.94%	2.086%
44	11.490	1451	1454	1458	rBV	174457	285235	3.41%	0.447%
45	11.537	1458	1462	1471	rVB7	266803	726509	8.69%	1.138%
46	12.131	1559	1563	1568	rBV8	144763	321428	3.85%	0.503%
47	12.255	1579	1584	1591	rBV3	643799	1487296	17.80%	2.329%
48	12.425	1610	1613	1618	rVB	429025	521128	6.24%	0.816%
49	12.978	1699	1707	1713	rBV	4852348	8356887	100.00%	13.087%
50	13.143	1732	1735	1737	rBV2	544741	740615	8.86%	1.160%
51	13.637	1816	1819	1823	rBV4	629116	888915	10.64%	1.392%
52	13.790	1842	1845	1850	rVB2	1268453	1489960	17.83%	2.333%
53	13.854	1854	1856	1861	rVB3	1182160	1400826	16.76%	2.194%
54	14.207	1912	1916	1922	rVB2	2538516	4877719	58.37%	7.638%
55	14.349	1936	1940	1942	rBV2	1510663	2512384	30.06%	3.934%
56	24.995	3747	3750	3763	rVB	763167	2160910	25.86%	3.384%

Sum of corrected areas: 63857765

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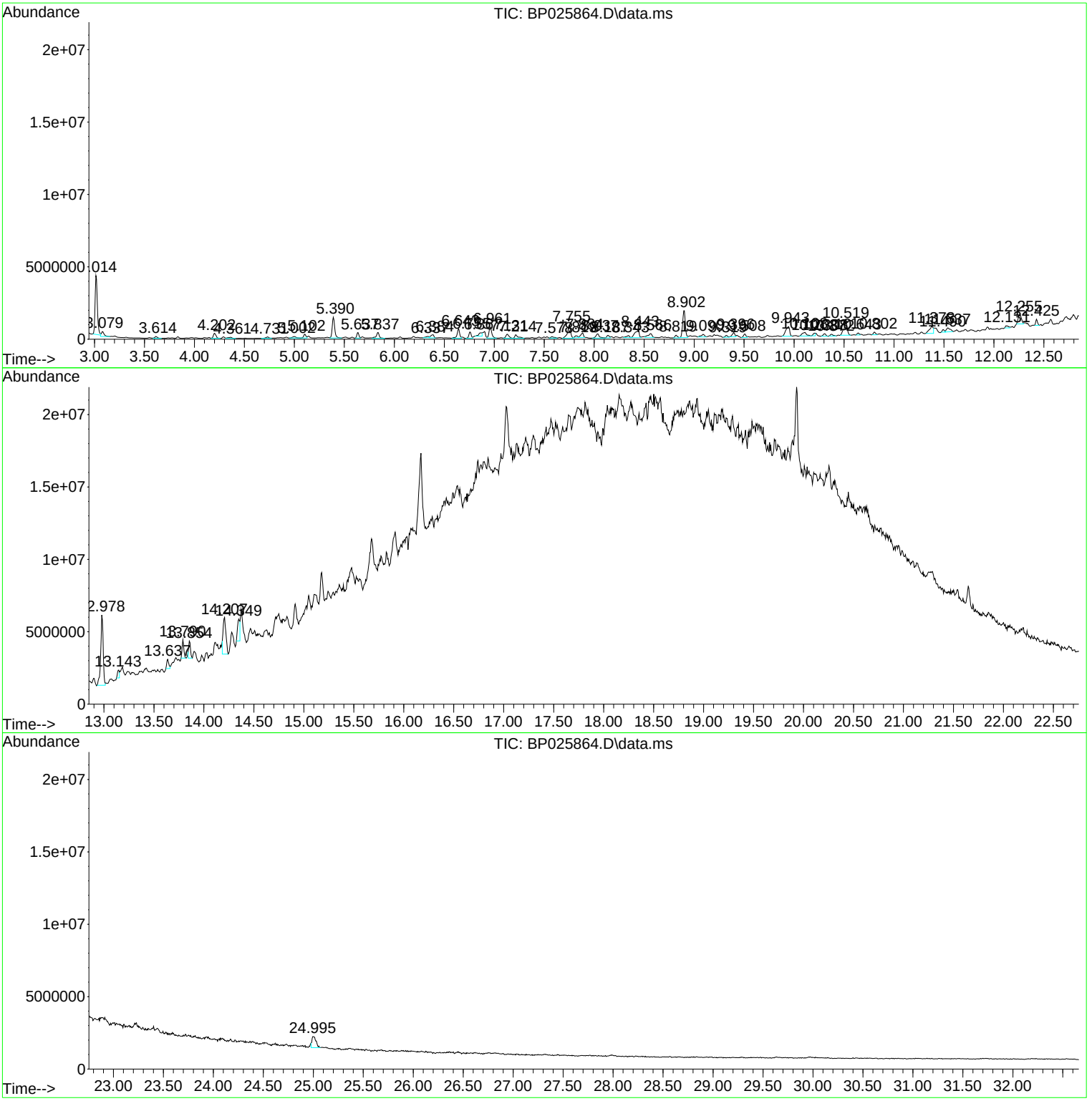
Acq On : 25 Sep 2025 19:32
Operator : CG/JU
Sample : Q3168-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TOTES COMP#1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP091225.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_P\Data\BP092525\
Data File : BP025864.D
Acq On : 25 Sep 2025 19:32
Operator : CG/JU
Sample : Q3168-05
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Instrument :
BNA_P
ClientSampleId :
TOTES COMP#1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP091225.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

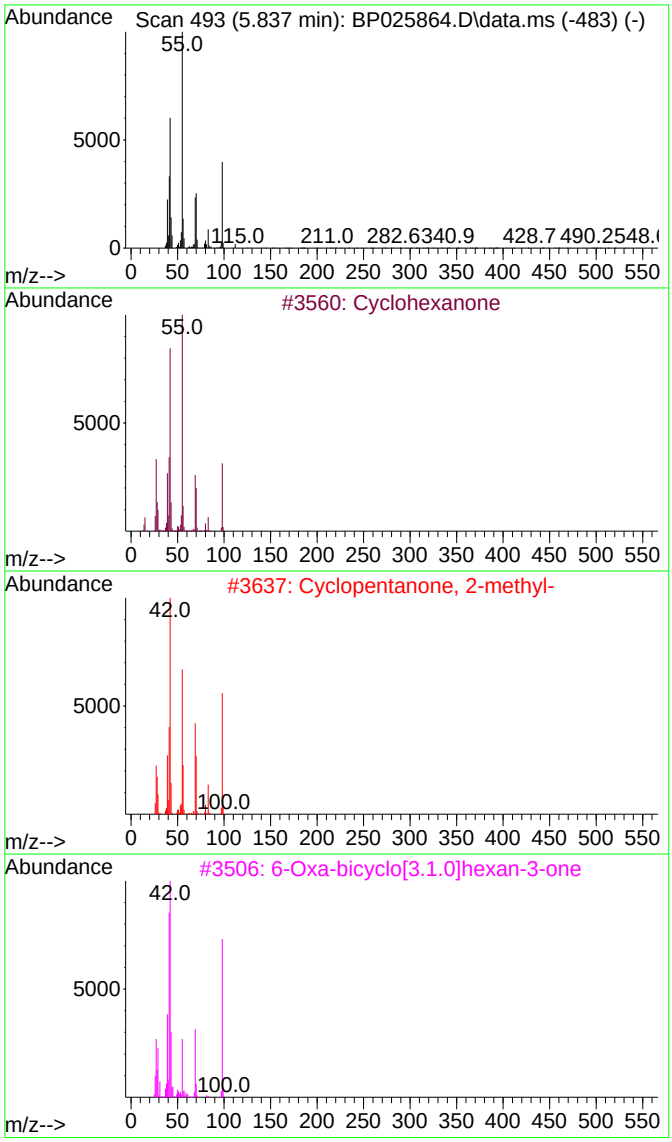
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

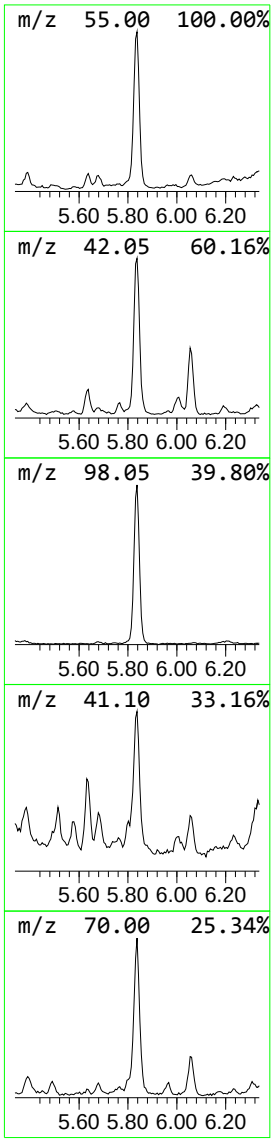
****

Peak Number 4 Cyclohexanone Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.837	8.41 ng	840858	1,4-Dichlorobenzene-d4	7.755

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexanone	98	C6H10O	000108-94-1	91
2	Cyclopentanone, 2-methyl-	98	C6H10O	001120-72-5	81
3	6-Oxa-bicyclo[3.1.0]hexan-3-one	98	C5H6O2	074017-10-0	47
4	2-Pentene, (Z)-	70	C5H10	000627-20-3	43
5	1,3-Cyclopentanedione	98	C5H6O2	003859-41-4	43





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP092525\
Data File : BP025864.D
Acq On : 25 Sep 2025 19:32
Operator : CG/JU
Sample : Q3168-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TOTES COMP#1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP091225.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

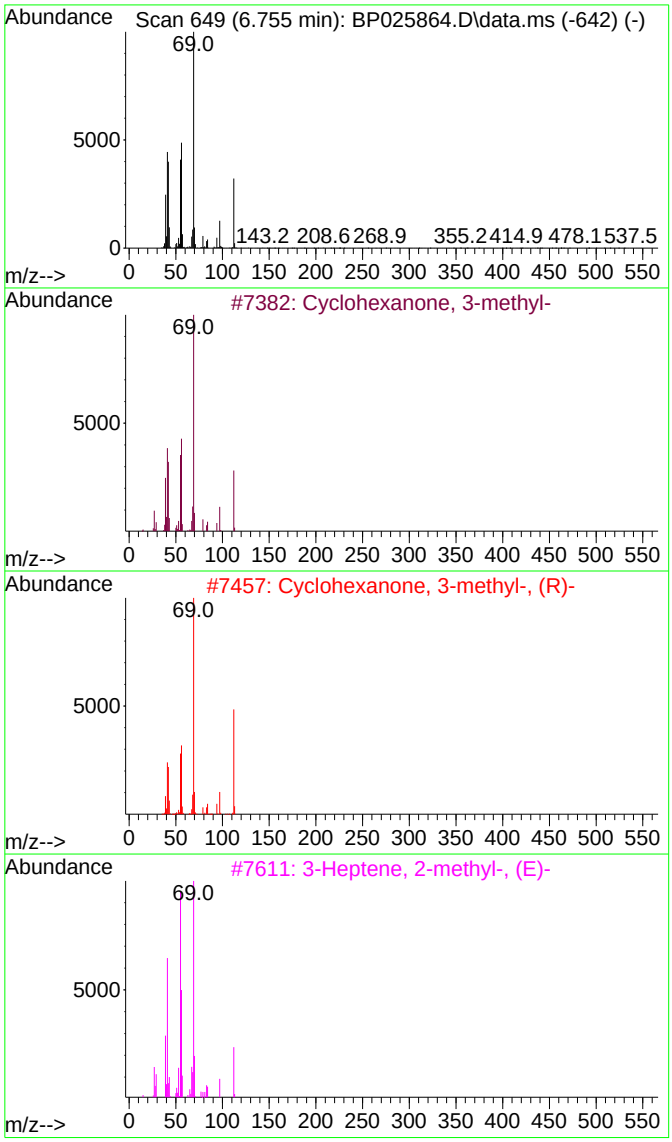
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

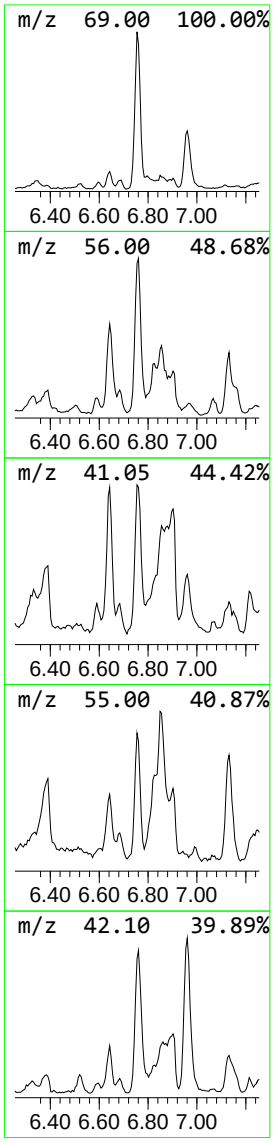
****

Peak Number 6 Cyclohexanone, 3-methyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.755	7.51 ng	750540	1,4-Dichlorobenzene-d4	7.755

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexanone, 3-methyl-	112	C7H12O	000591-24-2	94
2	Cyclohexanone, 3-methyl-, (R)-	112	C7H12O	013368-65-5	91
3	3-Heptene, 2-methyl-, (E)-	112	C8H16	000692-96-6	40
4	1-Hexene, 3,3-dimethyl-	112	C8H16	003404-77-1	37
5	2-Methyl-2-heptene	112	C8H16	000627-97-4	36





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP092525\
Data File : BP025864.D
Acq On : 25 Sep 2025 19:32
Operator : CG/JU
Sample : Q3168-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TOTES COMP#1

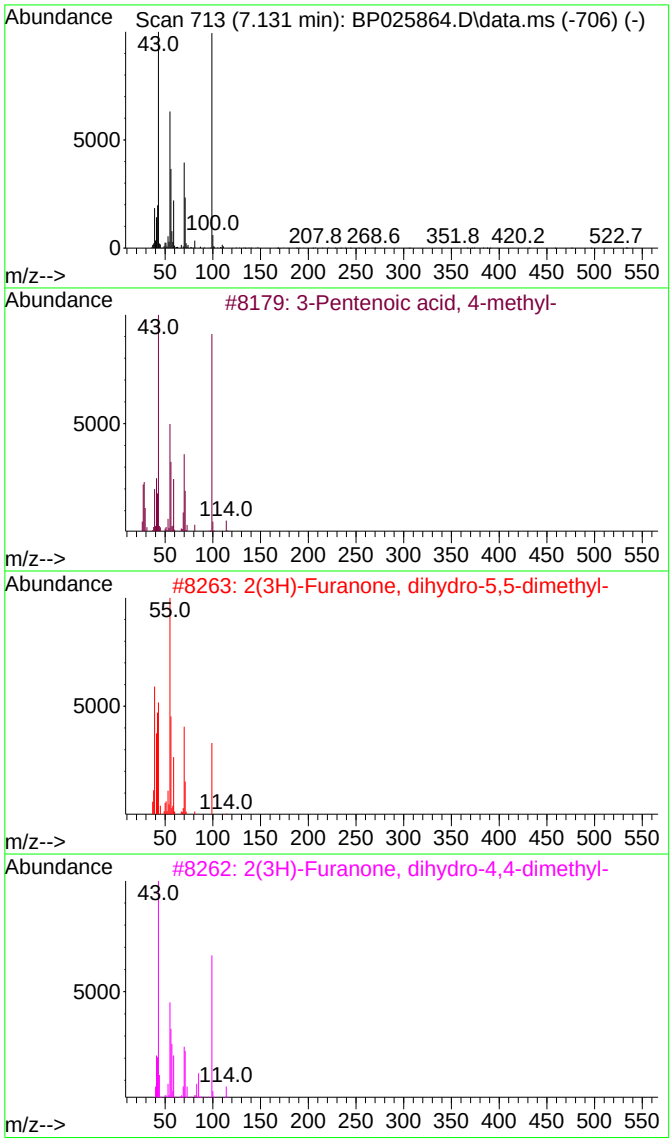
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP091225.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

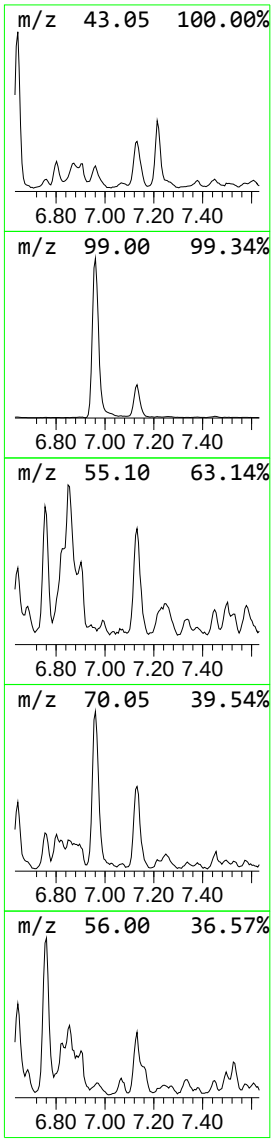
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 3-Pentenoic acid, 4-methyl- Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.131	5.70 ng	570453	1,4-Dichlorobenzene-d4	7.755

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Pentenoic acid, 4-methyl-	114	C6H10O2	000504-85-8	90
2	2(3H)-Furanone, dihydro-5,5-dime...	114	C6H10O2	003123-97-5	72
3	2(3H)-Furanone, dihydro-4,4-dime...	114	C6H10O2	013861-97-7	64
4	4H-Imidazol-4-one, 2-amino-1,5-d...	99	C3H5N3O	000503-86-6	50
5	Benzo[1,2,5]thiadiazole, 4-bromo...	376	C11H13BrN4O2S2	1000296-37-8	43





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP092525\
Data File : BP025864.D
Acq On : 25 Sep 2025 19:32
Operator : CG/JU
Sample : Q3168-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TOTES COMP#1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP091225.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

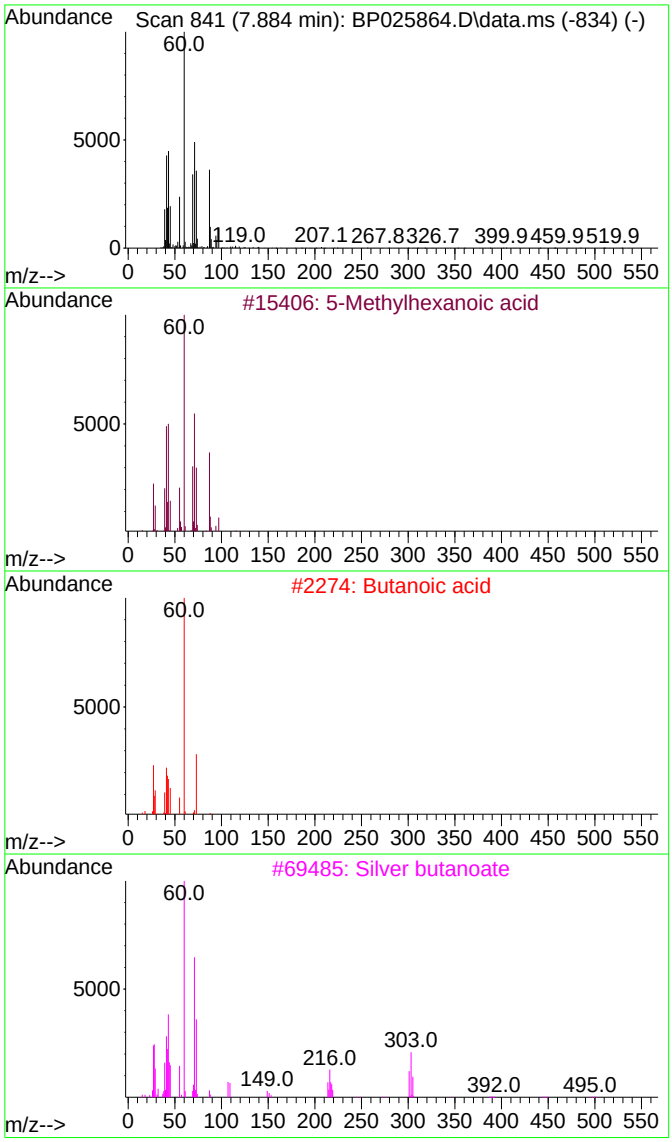
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

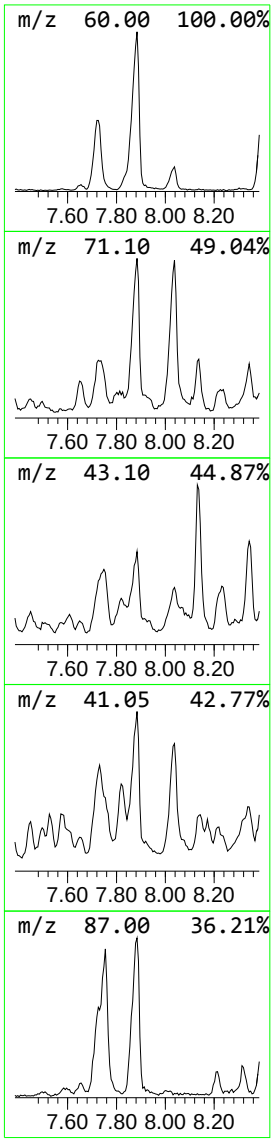
****

Peak Number 8 5-Methylhexanoic acid Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.884	6.01 ng	600513	1,4-Dichlorobenzene-d4	7.755

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Methylhexanoic acid	130	C7H14O2	000628-46-6	86
2	Butanoic acid	88	C4H8O2	000107-92-6	47
3	Silver butanoate	194	C4H7AgO2	005076-24-4	42
4	Pentanoic acid	102	C5H10O2	000109-52-4	37
5	3-Methyl-hexanoic acid	130	C7H14O2	1000365-65-4	36





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Acq On : 25 Sep 2025 19:32
Operator : CG/JU
Sample : Q3168-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TOTES COMP#1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP091225.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

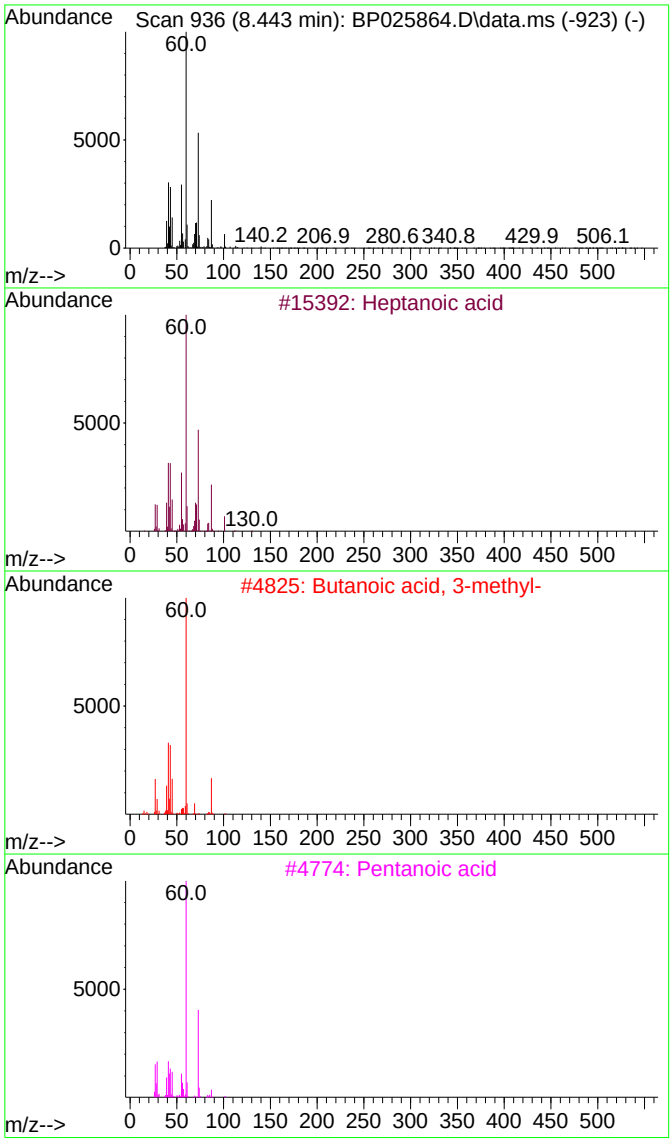
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

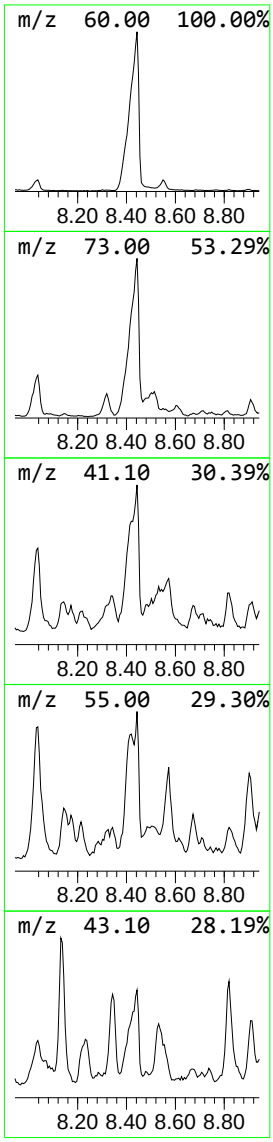
****

Peak Number 10 Heptanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.443	15.07 ng	1506700	1,4-Dichlorobenzene-d4	7.755

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptanoic acid	130	C7H14O2	000111-14-8	91
2	Butanoic acid, 3-methyl-	102	C5H10O2	000503-74-2	64
3	Pentanoic acid	102	C5H10O2	000109-52-4	64
4	Hexanoic acid	116	C6H12O2	000142-62-1	56
5	Butanoic acid	88	C4H8O2	000107-92-6	53





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Instrument :
BNA_P
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP091225.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

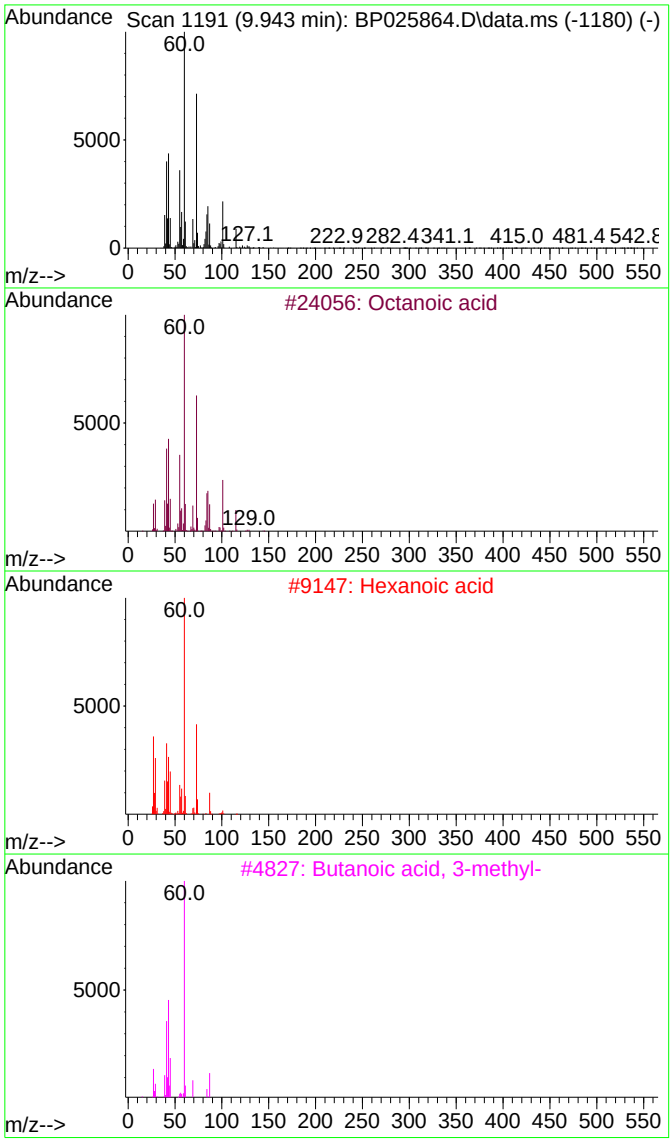
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

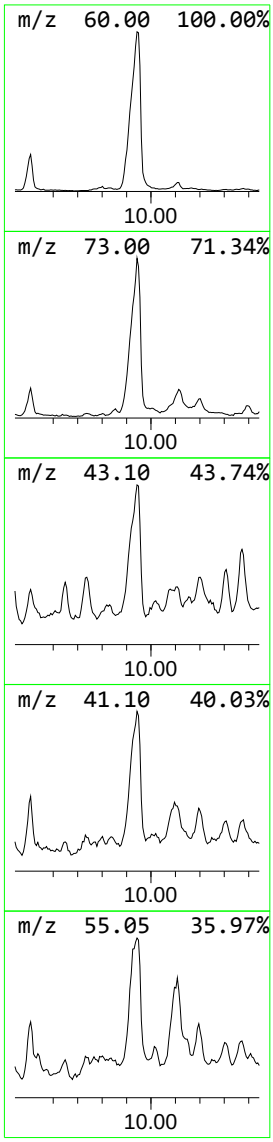
****

Peak Number 11 Octanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.943	16.18 ng	1811140	Naphthalene-d8	10.519

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octanoic acid	144	C8H16O2	000124-07-2	96
2	Hexanoic acid	116	C6H12O2	000142-62-1	53
3	Butanoic acid, 3-methyl-	102	C5H10O2	000503-74-2	47
4	Heptanoic acid	130	C7H14O2	000111-14-8	47
5	Pentanoic acid	102	C5H10O2	000109-52-4	47





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Data File : BP025864.D
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Operator : CG/JU
Sample : Q3168-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TOTES COMP#1

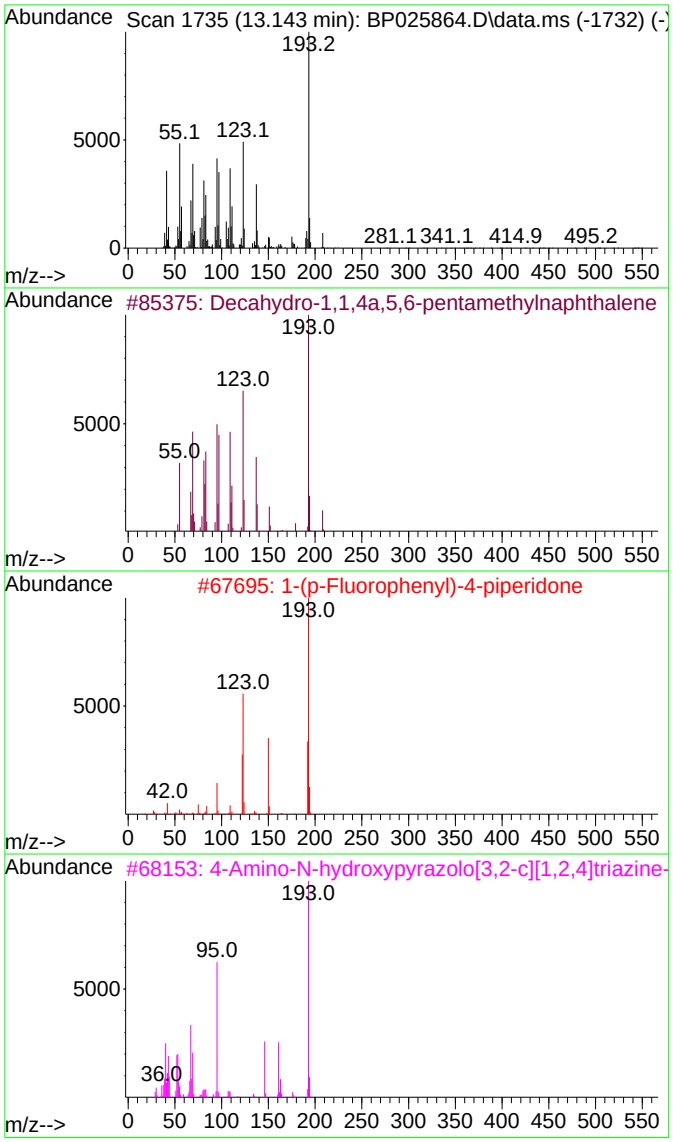
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP091225.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

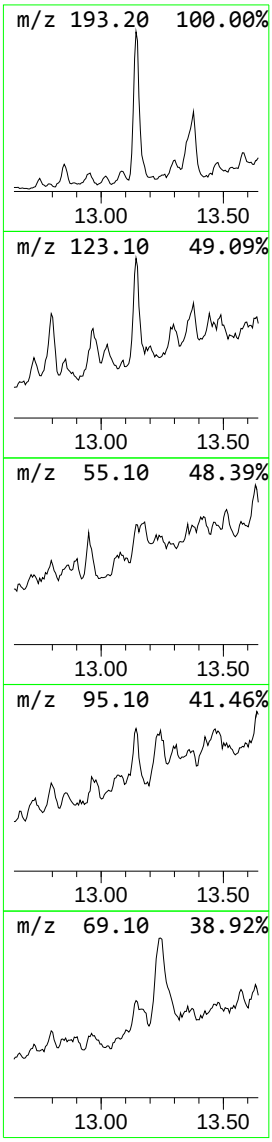
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 16 Decahydro-1,1,4a,5,6-pentam... Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.143	5.90 ng	740615	Acenaphthene-d10	14.372

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decahydro-1,1,4a,5,6-pentamethyl...	208	C15H28	080655-44-3	94
2	1-(p-Fluorophenyl)-4-piperidone	193	C11H12FNO	1000238-56-7	43
3	4-Amino-N-hydroxypyrazolo[3,2-c]...	193	C6H7N7O	1000443-50-2	38
4	2-Pentanone, 4-cyclohexylidene-3...	222	C15H26O	313253-65-5	35
5	2-Anthracenamine	193	C14H11N	000613-13-8	27





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP092525\
Data File : BP025864.D
Acq On : 25 Sep 2025 19:32
Operator : CG/JU
Sample : Q3168-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TOTES COMP#1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP091225.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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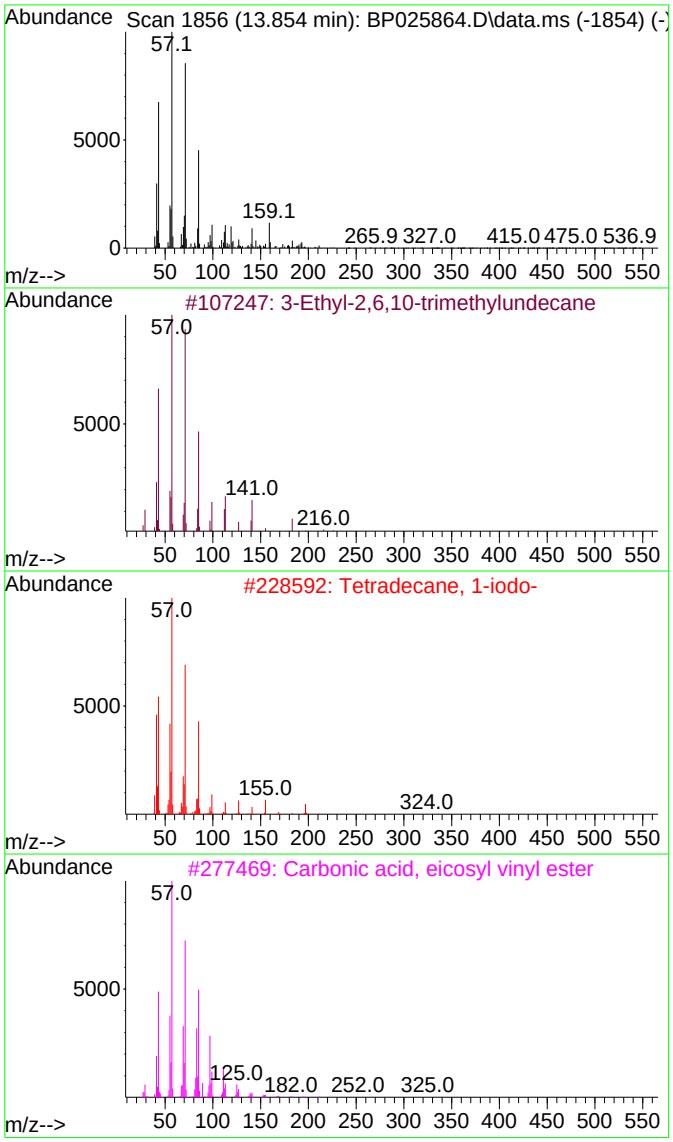
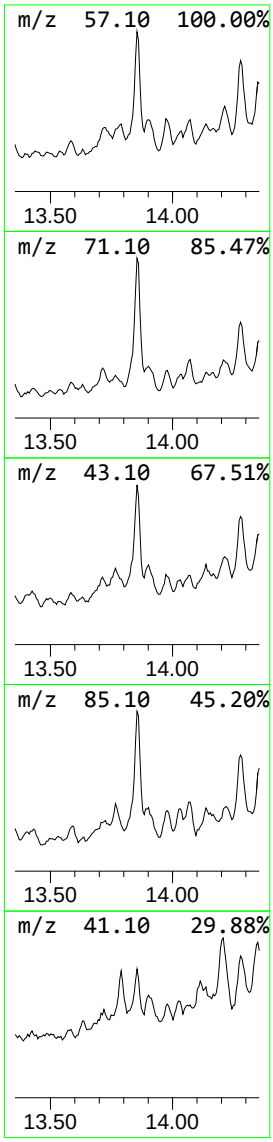
Peak Number 19 3-Ethyl-2,6,10-trimethylund... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.854	11.15 ng	1400830	Acenaphthene-d10	14.372

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Ethyl-2,6,10-trimethylundecane	226	C16H34	1000432-25-9	90
2	Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	80
3	Carbonic acid, eicosyl vinyl ester	368	C23H44O3	1000382-54-3	80
4	Tridecane, 5-propyl-	226	C16H34	055045-11-9	76
5	Hexadecane, 3-methyl-	240	C17H36	006418-43-5	72





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP092525\
Data File : BP025864.D
Acq On : 25 Sep 2025 19:32
Operator : CG/JU
Sample : Q3168-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TOTES COMP#1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP091225.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
Cyclohexanone	5.837	8.4	ng	840858	1	7.755	1999850	20.0
Cyclohexanone, ...	6.755	7.5	ng	750540	1	7.755	1999850	20.0
3-Pentenoic aci...	7.131	5.7	ng	570453	1	7.755	1999850	20.0
5-Methylhexanoi...	7.884	6.0	ng	600513	1	7.755	1999850	20.0
Heptanoic acid	8.443	15.1	ng	1506700	1	7.755	1999850	20.0
Octanoic acid	9.943	16.2	ng	1811140	2	10.519	2238830	20.0
Decahydro-1,1,4...	13.143	5.9	ng	740615	3	14.372	2512380	20.0
3-Ethyl-2,6,10-...	13.854	11.2	ng	1400830	3	14.372	2512380	20.0